HANDBOOK OF BOND DISSOCIATION ENERGIES IN ORGANIC COMPOUNDS

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To

Dr. Sidney W. Benson

who introduced me to the field of thermochemical kinetics
during my postdoctoral work at the University of Southern California

Preface

Three of the most fundamental concepts in organic chemistry are structure, energetics and reactivity, and their interrelationships. Sometimes, attempting to discover reliable data on bond dissociation energies (BDEs) or the strengths of chemical bonds may be a frustrating exercise, analogous to seeking a needle in a haystack.

I began to collect experimental and theoretical values for BDEs in 1990. Four years later, Dr. S.E. Stein of the National Institute of Standards and Technology (NIST) encouraged me to continue in this task, essential for chemical kinetics, free radical chemistry, organic thermochemistry, and physical organic chemistry.

A variety of methods exist for determining BDE values, but almost none are accurate to better than "chemical accuracy" (±1 kcal/mol, 1 calorie = 4.184 joules). The BDE values of many important compounds have been measured many times; for example, the C–H BDE in methane has been determined about 50 times since the 1930s. BDE values continue to be a source of lively controversy among scientists.

The data presented in this book are from experiments only, although theoretical calculations are very interesting. Collecting experimental BDE data has been like taking a class in the history of chemistry, with many prominent scientists having made significant contributions to the problems surrounding the BDEs. These include E.W.R. Steacie, L. Pauling, M. Szwarc, N.N. Semenov, and S.W. Benson.

The author is very happy to acknowledge the great help, encouragement, and discussions of many scientists in preparing this manuscript. These scientists are Professors S.W. Benson, F.W. Bordwell, Y.T. Lee, R.H. Byrne, A.M. Dean, J.F. Liebman, V.D. Parker, and I.R. Slagle (all of U.S.); P.D. Pacey, J.L. Holmes, D.A. Armstrong, and E. Tschuikow-Roux (all of Canada); J.A. Kerr, R. Walsh, and M.J. Pilling (all of U.K.); C. Rüchardt (Germany); K.D. King (Australia); X.Z. Zhao and J.P. Cheng (China); A.J. Colussi (Argentina); J.A.M. Simões (Portugal); J.A. Seetula (Finland); Drs. S.E. Stein and W. Tsang (NIST); T.J. Wallington (Ford Motor Company); M. Tirtowidjojo (Dow Chemical Company); K.U. Ingold, D.D.M. Wayner (NRC, Canada); and E.T. Denisov (Russia). I also would like to thank the reviewers for their suggestions and comments.

All comments and suggestions are welcomed. Anyone may contact me by e-mail at luo@molenergetics.com.

Yu-Ran Luo

List of notations and abbreviations

AE	appearance energy measurements
AP	appearance potentials
AOP	acidity–oxidation potential measurements
BDE	bond dissociation energy (or enthalpy)
CID	collision-induced dissociation
detect.	detection
DH^{o}	i.e., BDE, where H emphasizes the BDE is an enthalpy change of thermochemistry
electrochem.	electrochemical technique
EA	electron affinity measurements
EPR	electron paramagnetic resonance spectrometry
ESR	electron spin resonance spectrometry
FT-ICR	Fourier transform ICR
FT-MS	Fourier transform mass spectrometry
FT-IR	Fourier transform infrared spectrometry
GPA	gas-phase acidity measurements
GC	gas chromatographic analysis
HPLC	high performance liquid chromatography
ICR	ion cyclotron resonance spectrometry
IE	electron impact method
IR	infrared spectrometry
MS	mass spectrometry
NMR	nuclear magnetic resonance spectrometry
PAC	photoacoustic calorimetry
PIMS	photoionization mass spectrometry
photobromin.	photobromination
photochlorin.	photochlorination
photodetach.	photodetachment
photodissocn.	photodissociation
photoelectr.	photoelectron
re-anal.	re-analysis of experimental data, i.e., revised
re-cal.	re-calculated BDEs from experimental data, i.e., revised
recommend.	recommended value
spectrom.	spectrometry
SPST	single-pulse shock tube technique

TR-PAC	time-resolved photoacoustic calorimetry
UV/VIS	ultraviolet and visible spectrometry detection
VLPP	very low pressure pyrolysis technique
VLPR	very low pressure reactor method

Contents

chapter one

Introduction

1.1 A database of the BDEs

Chemistry and biochemistry are based on the concept of chemical bonds. The breaking and making of chemical bonds are involved in most chemical reactions. Chemists, biochemists, and chemical engineers thus need a complete database of the experimental data of bond dissociation energies (BDEs).

This book contains the experimental BDE data of **2700** bonds in **2400** organic compounds. It is the first comprehensive book on experimental BDE data. It is very helpful to end users searching for BDE data.

1.2 What is the BDE?

The homolytic BDE is defined as the enthalpy change in the following fission:

$$R\text{–}X \rightarrow R + X \tag{1.1}$$

The BDE, $DH^o(R\text{–}X)$, of an R–X bond is derived in the usual way from heats of formation of the species involved in the previous reaction:

$$DH^o(R\text{–}X) = \Delta_f H^o(R) + \Delta_f H^o(X) - \Delta_f H^o(RX) \tag{1.2}$$

Here $\Delta_f H^o$ represents the heats of formation of the respective species in the ideal gas state at standard pressure and a reference temperature of 298.15 K. The BDE is also called the bond dissociation enthalpy.

Today, heats of formation, $\Delta_f H^o(RX)$, of about **four thousand** organic compounds are known. Most of them are available in the following publications: 1994FRE/KAB, 1994PED, 1994GUR/VEY, 1989COX/WAG, 1988LIA/BAR, 1986PED/NAY, and http://webbook.nist.gov. The experimental uncertainty of heats of formation of organic compounds is generally within the "chemical accuracy" (±1 kcal/mol, 1 calorie = 4.184 joules). From Equation 1.2, measurements of BDEs are equivalent to measurements of heats of formation of free radicals, and vice versa. Experimental BDEs can be determined directly, and can be derived from Equation 1.2. For example, we may derive the BDE values of CH_3–X and C_2H_5–X, where X = H, F, Cl, Br, I, OH, SH, NH_2, CN, NO, NO_2, CH_3, and C_2H_5, if $\Delta_f H^o(CH_3)$ and $\Delta_f H^o(C_2H_5)$ are known.

The number of organic compounds confirmed is about **twenty million**. We must estimate the heats of formation of organic compounds and BDEs using *ab initio* MO theory,

density functional theory (DFT), semiempirical methods (such as PM3, AM1), molecular mechanics, group additivity, and others. The theoretical calculations are very interesting, but calculated BDEs are not included in this book.

1.3 Why we need reliable BDEs

The BDE measurements of organic compounds started in the 1930s. Szwarc first summarized many experimental BDEs in organic compounds (1950SZW). The earlier experimental data were collected by several publications: 1946STE, 1958COT, 1958SEM, 1962MOR, and 1966VED/GUR. Since then, almost all of these data have been updated. For example, the H–C BDE value in benzene increases to 111.2 ± 0.8 kcal/mol (1994BER/ELL) from 102 kcal/mol (1966VED/GUR).

The equilibrium constant K_{eq} is very sensitive to any error in the BDEs. An error of 1, 2, or 3 kcal leads to an error of a factor of 5.4, 29.2, or 158, respectively, in the equilibrium constant K_{eq} at 298 K! The currently experimental uncertainty of the absolute majority of BDE data is within 1 to 2 kcal/mol, which means the uncertainty is more than "chemical accuracy" (±1 kcal/mol). Experimental BDE values thus will continue to be a source of lively controversy among scientists now and in the foreseeable future.

Several senior reviewers made efforts to update known BDEs as soon as possible, such as 1966KER, 1969GOL/BEN, 1970ONE/BEN, 1978BEN, 1982MCM/GOL, 1988COL, 1994BER/ELL, 1996TSA, and 1999COH. However, the number of experimental BDEs is increasing sharply. For example, the *CRC Handbook of Chemistry and Physics* (2002CRC) collected the BDEs of about **400** bonds in organic compounds. Now we have collected experimental data for more than **2700** bonds. Chemists, biochemists, and chemical engineers need a new publication which completely compiles the BDEs available.

By the way, a good BDE database of diatomic molecules can be found in Section 9 of the *CRC Handbook of Chemistry and Physics* (2002CRC), which collects over **800** data. BDEs of diatomic and smaller molecules can also be derived by using the *NIST-JANAF Thermochemical Table* (1998CHA).

1.4 Scope of this book

Experimental BDEs of many important organic compounds have been remeasured many times. A typical example is C–H BDE in methane. It has been reported up to 50 times since the 1930s, and the value spreads from an early 98 kcal/mol to the current 105 kcal/mol. We have collected all experimental data; however, it is not necessary to copy all of the data into this book, because most users are concerned with reliable experimental values only.

This book will present recent experimental data for the given bonds, a maximum of five values for each bond. Which is the most reliable or best data for the BDEs? It is hard to answer this question. Recent measurements are likely to be more reliable generally. Readers may search more experimental data by using the references listed.

The BDEs have been tabulated based on the center atom in the radicals. They are distinguished by C–X, O–X, N–X, S–X, Si–X, Ge–X, Sn–X, P–X, and Se–X BDEs, and are organized in Chapters Three through Nine.

The BDE data in some but not all inorganic compounds are listed in Chapter Ten. At present, this book does not collect the BDE data in metallorganic compounds. A great number of experimental data for ionic species are beyond the scope of this book, because

these data have been available in other databases: 1988LIA/BAR and http://webbook.nist.gov.

1.5 On energy units

The SI unit of energy is joule (1 calorie = 4.184 joules). There are three options for energy units: (1) joule only, (2) calories only, and (3) both units. Using both units is a better choice.

Why? There are two reasons: (1) most heats of formation of radicals and BDEs used to be measured in kcal/mol and (2) the range of the BDE values for common organic species is from about 40 (as RO–OR) to 110 (as H–C_6H_5, H–C_2H_3) kcal/mol. As you know, a lower number is easy to remember in everyday life; it is the same in science. For example, we may easily remember 105.0 kcal/mol of H–CH_3 BDE rather than 439.3 kJ/mol.

1.6 How to search for BDEs in this book

We encountered a great number of experimental BDEs from over 1000 publications. The data are like "goods" in a large department store: they should be organized on different "shelves" or locations for our "shopping." In this book, these data are managed in various categories. The chemical bonds with most similar structural environments are assembled in tables: "goods shelves." There are 49 tables for BDE data in this book. All tabulated values of the BDEs are systematized by the following seven orders:

1. **Bond class**, such as C–H, C–C, C–O, C–N, C–S, C–F, C–Cl, C–Br, C–I, and so on.
2. **Heteroatom(s) and functional group(s) at α-position** (relative to the broken bond), such as O, CO, C(O)O, N, CN, NO, NO_2, NN, S, SO, SO_2, and more. The heteroatom(s) and functional group(s) have significant influence on the BDEs. Organic chemistry is usually organized by the concept of functional groups. Therefore, users must first figure out heteroatom(s) and functional group(s) before searching the data. For example:
   - The primary C–H BDE in $C_6H_5CH_2$–**H** is listed in Table 3.4. In this book, the **boldface** emphasizes the dissociated atom or group.
   - The secondary C–H BDE in Ph**C**$\mathbf{H}_2$$COCH_3$ is listed in Table 3.6.1. There is a CO group at the α-position of the C–H bond.
   - The secondary C–H BDE in PhCOC$\mathbf{H}_2$$NMe_2$ is listed in Table 3.6.3. There are a CO group and an N atom at the α-position of the C–H bond.
   - The secondary C–H BDE in PhCOC$\mathbf{H}_2$$SO_2$Ph is listed in Table 3.6.4. There are a CO group and a SO_2 group at the α-position of the C–H bond.
3. **Bond order** (triple, double, and single) and the **bond degree** (primary, secondary, or tertiary). The compounds with triple bond and primary BDEs are listed first.
4. **Saturated or unsaturated** compounds. Saturated ones are listed first.
5. **Molecular size**. The BDEs of smaller molecules are arranged first.
6. **Molecular shape (chain or cyclic)**. The BDEs of chain molecules are arranged first.
7. While **substituent(s)-containing**, please first search the bonds in the parent molecules. For example, the C–H BDEs in substituted toluene are listed under $C_6H_5CH_2$–**H**.

Two indexes may also help your search, one of compound classes and the other of compound names.

1.7 *How to use the tables of the BDE data*

All BDE data are filed into 49 different tables. How can you find the BDEs? Let us see a first example, the C–H BDE in methane:

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
methane	(1) **105.0±0.1**	439.3±0.4	(1) VLPP	(1) 1987DOB/BEN
	(2) 105.3±0.7	440.6±2.9	(2) PIMS detection	(2) 1988RUS/SEE(b)
CH_3–**H**	(3) 104.8±0.2	438.5±0.8	(3) Spectrometric detection	(3) 1988RUS/SEE
$\Delta_f H^o(R)$ = 35.06±0.1 (146.69±0.4)	(4) 105.3±0.6	440.6±2.5	(4) Resonance detection	(4) 1991NIC/DIJ
	(5) 104.99±0.03	439.28±0.13	(5) AE, revised	(5) 1999RUS/LIT

The first column in this table shows the broken bonds. The **boldface** emphasizes the dissociated atom or group; here the H is **boldfaced**. For example, $CH_3C\mathbf{H}_2CH_2CH_3$ shows a secondary C–H bond in n-butane is broken; $(CH_3C\mathbf{H}_2)_3N$ shows a secondary C–H bond in triethylamine is broken. All expressions are similar. The heat of formation of free radicals is shown in this cell. Chapter Eleven includes tables of all $\Delta_f H^o(R)$.

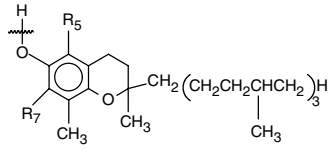
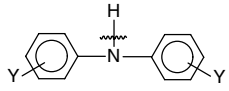
The second column shows the experimental values of BDEs for the given bond. The numbers (1), (2), (3), (4), and (5) show five different resources or references. The recommended value is emphasized by **boldface**.

The third column shows various experimental methods for the relevant BDE value. For an explanation of terms, see the Notations and Abbreviations list in this book.

The fourth column shows the references for the given experimental methods and for the relevant BDE value. A maximum of five values are provided. This is sufficient for most users. Readers can search for more references while using the references here.

Following are another three examples:

1. The C–O BDE in methoxybenzene or anisole. The experimental data of BDE(C–O) are from four different methods. The first three values are contributed from independent measurements of different research groups. The last one is derived by Equation 1.2, in which heats of formation of the parent molecules are taken from the given reference, and heats of formation of atoms and radicals are taken from Chapter Eleven.
2. The weakest H–O BDEs in four tocopherols (vitamin E). They emphasize the difference of experimental H–O BDEs in gas phase and in liquid phase.
3. The H–N BDEs in substituted diphenylamine. They show the effect of various remote substituents Y on the H–N BDEs.

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
methoxybenzene or anisole	(1) 64.8	271.1	(1) VLPP	(1) 1989SUR/KAF
	(2) 65.2	272.8	(2) Tubular flow reactor	(2) 1993ARE/LOU
CH_3–OC_6H_5	(3) 65.3	273.2	(3) VLPP	(3) 2001PRA/HEE
	(4) **64.2±1.7**	**268.6±7.1**	(4) Derived from $\Delta_f H^o$ in ref.	(4) 1986PED/NAY
α-tocopherol				
				
$R_5 = R_7 = CH_3$ (vitamin E)	(1) 80.4	336.4	(1) Estimated by rate constants	(1) 1985BUR/DOB
	(2) 78.9	330.1	(2) EPR	(2) 1992JAC/HOS
	(3) 78.9	330.1	(3) EPR	(3) 1994LUC/PED
	(4) 80.9±1.0, in solution	338.5±4.2	(4) AOP	(4) 1996BOR/LIU
	(5) **79.3**, in solution	**331.8**	(5) APC	(5) 1996WAY/LUS
	(5) **77.3**, in gas	**323.4**		
δ-tocopherol $R_5 = R_7 = H$	(5) 82.2, in solution	343.9		
	(5) 80.2, in gas	335.6		
	(6) 81.9	342.8	(6) Correlation	(6) 2000DEN/DEN
β-tocopherol $R_5 = CH_3$, $R_7 = H$	(6) 80.2	335.6		
γ-tocopherol $R_5 = H$, $R_7 = CH_3$	(6) 80.1	335.1		
diphenylamine, substituted				
				

(continued)

Table (continued)

The broken bonds (**boldface** – dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
Y = p-Br	(1) 88.1	368.6	(1) AOP	(1) 1993BOR/ZHA
	(2) 87.0	364.2	(2) Correlation	(2) 2000DEN/DEN
p-MeO	(1) 84.2	352.3		
	(2) 83.3	348.6		
	(4) 81.8	342.2		
p-Me	(2) 85.4	357.5		
	(3) 86.3 in sol.	361.1 in sol.	(3) PAC	(3) 1997MAC/WAY
	(3) **86.2** in gas	**360.7** in gas		
	(4) 83.3	348.5	(4) EPR	(4) 2002PRA/DIL
p-tBu	(2) 85.8	358.8		
p-$N(CH_3)_2$	(4) 79.5	332.6		

chapter two

Experimental methods for measuring BDEs

The object of most end users is to find reliable data. However, it is very helpful if the users know the sources of experimental BDE data.

A very concise description of experimental methods is summarized below. It provides main methods, measured quantities, applications, and references. It is hoped that it may help the reader to better interpret the tables of BDE data from Chapters Three through Ten.

Table 2.1 A Summary of Main Experimental Methods for Measuring BDEs

Experimental Methods	Measured Quantities	Applications	References
Spectrometry	Spacing of vibrational energy levels	Diatomic molecules in gas phase	(1) 1968GAY (2) 1970DAR (3) 1979HUB/HER
Pyrolysis kinetics, including	Concentration of atoms, free radicals, and molecules vs. time at different temperatures, using various detecting techniques, such as GC, HPLC, MS, FT-IR, UV/VIS, EPR, NMR, resonance fluorescence, chemiluminescence, etc.	Species in gas and solution phase	
• Toluene carrier tech			1950SZW
• Very low pressure pyrolysis (VLPP)			(1) 1973GOL/SPO (2) 1979ROS/KIN (3) 1982MCM/GOL
• Shock tubes			(1) 1992DOU/MAC (2) 1997KIE/ZHA
• Single-pulse shock tubes (SPST)			(1) 1981TSA (2) 1999TSA
• Laser-powered pyrolysis			(1) 1982MCM/LEW (2) 1984LEW/GOL

(continued)

Table 2.1 (continued) A Summary of Main Experimental Methods for Measuring BDEs

Experimental Methods	Measured Quantities	Applications	References
Chemical equilibrium and kinetics	Concentration of atoms, free radicals, and molecules at one or several temperatures, using various detecting methods	Species in gas and solution phase	(1) 1966KER (2) 1977KER (3) 1982CAS/GRI (4) 1982MCM/GOL (5) 1984PAC/WIL (6) 1990KOE/SCO (7) 1990HAL (8) 1992WAL (9) 1994BER/ELL
	Correlation between BDEs and rate constants or activation energies		(1) 1966KER (2) 1978KAT/RAJ (3) 2000DEN/DEN
Photolysis, including	Concentration at one or several temperatures, using various analytical methods	Species in gas and solution phase	
• UV			(1) 1971LAU/OKA (2) 1995BOY/NOZ
• Radiolysis			(1) 1990LIN/SHE (2) 2001DAS
• Laser			(1) 1987CHU/FOL (2) 1988PEN/CAO (3) 1997BEC/CAR
• Photosensitized			1967LOU/LAI
Mass spectrometry (MS), including	Measure the given quantities and describe their correlation with BDEs	Species in gas phase	2001ERV
• Electron impact	Ion intensities vs. electron energy		(1) 1979BER (2) 1984HOL/LOS (3) 1992HOL
• Guided ion beam	Ion intensities vs. ion kinetic energy		(1) 1995ARM (2) 1998DET/ERV
• High pressure	Ion intensities vs. temperature		(1) 1994BUS/KEM (2) 1994BOW (3) 1999MCM

• Ion cyclotron resonance (ICR)	Ion intensities vs. time, vs. electron or photon energy		(1) 1980DEF/MCI (2) 2000BOR/ING (3) 1999ABB/NOT
• High temperature	Ion intensities vs. temperature		1984MAR
• Photoionization (PIMS)	Ion intensities vs. photon energy		(1) 1994BER/ELL (2) 1994BAR
• Pulsed high pressure	Ion intensities at one or several temperatures		(1) 1989MEO (2) 1993SHA/KEB
• Kinetic method	Ion intensities		1994COO/PAT
• Kinetic energy release distributions	Ion intensities vs. product kinetic energy		1992BEA
Photospectrometry, including	Measure the given quantities and describe their correlation with BDEs	Species in gas phase	
• Photoelectron	Electron count vs. electron kinetic energy		(1) 1984MEA (2) 1994BER/ELL
• Electron photo-detachment	Ion intensities vs. photon energy		(1) 1987WET/BRA (2) 1989CHE/ALB
• Flowing afterglow	Ion intensities vs. time, or vs. ion kinetic energy		(1) 1992SQU (2) 1994BER/ELL
• Collision-induced dissociation	Collision energy vs. cross section		(3) 1994WEN/SQU (4) 2001HAM/WEN
Electrochemical, including acidities and oxidation potentials (AOP)	Acidity, reversible redox potentials	Species in solution	(1) 1993BOR/ZHA (2) 1993WAY/PAR (3) 1993ARN/FLO (4) 1995BOR/SAT
Photoacoustic calorimetry (PAC)	Amplitude of photoacoustic signal and solution transmittance	Species in solution	(1) 1989KAM/GIL (2) 1994PET (3) 1999LAA/MUL (4) 1999SAN/LAG
	Time-resolved PAC		(5) 2002SAN/MUR

chapter three

Tabulated BDEs of C–H bonds

3.1 Chain saturated hydrocarbons

Table 3.1 C-H BDEs in Chain Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
methane	(1) **105.0±0.1**	**439.3±0.4**	(1) VLPP	(1) 1987DOB/BEN
CH_3–**H**	(2) 105.3±0.7	440.6±2.9	(2) PIMS detection	(2) 1988RUS/SEE(b)
$\Delta_f H^o(R)$ = 35.06±0.1 (146.69±0.4)	(3) 104.8±0.2	438.5±0.8	(3) Spectrometric detection	(3) 1990SEE/RUS
	(4) 105.3±0.6	440.6±2.5	(4) Resonance fluorescence detection	(4) 1991NIC/DIJ
	(5) 104.99±0.03	439.28±0.13	(5) AE, revised	(5) 1999RUS/LIT
ethane	(1) 100.5±0.5	420.5±2.1	(1) Kinetics	(1) 1984PAC/WIN
CH_3CH_2–**H**	(2) 100.5±0.5	420.5±2.1	(2) Resonance fluorescence detection	(2) 1986BRO/LIG
$\Delta_f H^o(R)$ = 28.4±0.3 (118.8±1.3)	(3) 100.8±0.7	421.7±2.9	(3) PIMS detection	(3) 1988RUS/SEE(b)
	(4) 101.0±0.4	422.6±1.7	(4) PIMS detection	(4) 1992SEA/PIL
	(5) **100.5±0.3**	**420.5±1.3**	(5) VLPP	(5) 1997DOB/BEN
propane	(1) 99.9±1.0	418.0±4.2	(1) Radical buffer	(1) 1982CAS/GRI
$CH_3CH_2CH_2$–**H**	(2) 99.8±2	417.6±8.4	(2) AE	(2) 1992HOL

(continued)

Table 3.1 (continued) C–H BDEs in Chain Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$\Delta_f H^o(R) = 23.8 \pm 0.5$ (100 ± 2)	(3) **100.9±0.5**	**422.2±2.1**	(3) SPST	(3) 1996TSA
	(4) 101.2±0.5	423.4±2.1	(4) PIMS detection	(4) 1997SEE/SLA
propane $CH_3C\mathbf{H}_2CH_3$ $\Delta_f H^o(R) = 21.0 \pm 0.7$ (88 ± 3)	(1) **98.1±0.7**	**410.5±2.9**	(1) PIMS detection	(1) 1988RUS/SEE(b)
	(2) 98.9±0.6	413.8±2.5	(2) PIMS detection	(2) 1990SEE/RUS
	(3) 98.6±0.4	412.5±1.7	(3) PIMS detection	(3) 1992SEA/PIL
	(4) 97.8±0.5	409.2±2.1	(4) PIMS detection	(4) 1997SEE/SLA
	(5) 97.4±1.0	407.5±4.2	(5) SPST	(5) 1999TSA
butane $CH_3CH_2CH_2CH_2$–**H** $\Delta_f H^o(R) = 18.6 \pm 0.5$ (77.8±2.1)	(1) 101±2	422.6±8.4	(1) Electron impact	(1) 1958COT
	(2) 100.2	419.2	(2) AE	(2) 1988HOL/LOS
	(3) **100.7**	**421.3**	(3) SPST	(3) 1990WAL/TSA
	(4) 101.7± 0.5	425.5±2.1	(4) PIMS detection	(4) 1997SEE/SLA
butane $CH_3C\mathbf{H}_2CH_2CH_3$ $\Delta_f H^o(R) = 16.2 \pm 0.5$ (67.8±2.1)	(1) 99.1±0.4	414.6±1.7	(1) PIMS detection	(1) 1990SEE/RUS
	(2) **98.3±0.5**	**411.1±2.2**	(2) Resonance fluorescence detection	(2) 1992SEA/PIL
	(3) 98.6±0.5	412.5±2.1	(3) Review	(3) 1996TSA
	(4) 98.3±0.5	411.3±2.1	(4) PIMS	(4) 1997SEE/SLA
	(5) 97.4±1.0	407.5±4.2	(5) SPST	(5) 1999TSA
isobutane $(CH_3)_2CHCH_2$–**H**	(1) **100.2±1**	**419.2±4.2**	(1) Exp. analysis	(1) 1976BEN
	(2) 99.3±2	415.5±8.4	(2) AE	(2) 1992HOL

$\Delta_f H^o(R) = 16.7 \pm 1.0$ (70±4)	(3) 101.6±0.5	425.1±2.1	(3) PIMS detection	(3) 1997SEE/SLA
	(4) 100.9±1	422.0±4.2	(4) SPST	(4) 1999TSA
isobutane $(CH_3)_3C–\mathbf{H}$ $\Delta_f H^o(R) = 11.5 \pm 0.7$ (48±3)	(1) 95.6±0.7	400.0±2.9	(1) SPST	(1) 1985TSA
	(2) 95.0	397.5	(2) VLPP	(2) 1987BEN/KON
	(3) 95.5±0.7	399.6±2.9	(3) Resonance fluorescence detection	(3) 1991SEA/PIL
	(4) 95.5±0.3	399.6±1.3	(4) Resonance fluorescence detection	(4) 1992SEA/PIL
	(5) **95.7±0.7**	**400.4±2.9**	(5) Recommend.	(5) 1996TSA
neopentane $(CH_3)_3CCH_2–\mathbf{H}$ $\Delta_f H^o(R) = 8.7 \pm 2$ (36.4±8.2)	(1) 99.4±1	415.9±4.2	(1) Polanyi correlation	(1) 1966KER
	(2) **100.3±1**	**419.7±4.2**	(2) Kinetics	(2) 1969LAR/HAR
	(3) 99.4±1	415.9±4.2	(3) SPST	(3) 1969TSA
	(4) 101.0±2	422.6±8.4	(4) Review	(4) 1982MCM/GOL
	(5) 101.1	423	(5) Laser flash photolysis	(5) 2001IMR/DOB
2-methylbutane $(CH_3CH_2)C\mathbf{H}(CH_3)_2$ $\Delta_f H^o(R) = 7$ (29)	(1) 91.6±2	383.3±8.4	(1) SPST	(1) 1969TSA
	(2) 96.5±1	403.8±4.2	(2) SPST	(2) 1981TSA
	(3) 92.6	387.4	(3) Photoelectron spectroscopy	(3) 1986KRU/BEA
	(4) **95.8**	**400.8**	(4) SPST	(4) 1999TSA
pentane $nC_5H_{11}–\mathbf{H}$ $\Delta_f H^o(R) = 13$ (54.4)	100.2	419.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentane $CH_3C\mathbf{H}_2(CH_2)_2CH_3$ $\Delta_f H^o(R) = 12$ (50.2)	99.2	415.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 3.1 (continued) C–H BDEs in Chain Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-methylpentane $(C_3H_7)C\mathbf{H}(CH_3)_2$ $\Delta_f H^o(R) = 0.8 \pm 2$ (3.3±8.2)	94.7±2	396.2±8.4	Pyrolysis	1983SER/GOR
2,3-dimethylbutane $CH_3CH(CH_3)C\mathbf{H}(CH_3)_2$ $\Delta_f H^o(R) = 0.7 \pm 2.4$ (3.1±10)	95.4±3.1	399.2±13.0	Equilibrium study	2000KIR/KOR
hexane nC_6H_{13}–**H** $\Delta_f H^o(R) = 8$ (33.5)	99.0	414.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
hexane $CH_3C\mathbf{H}_2(CH_2)_3CH_3$ $\Delta_f H^o(R) = 7$ (29.3)	98.0	410.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
heptane $CH_3C\mathbf{H}_2(CH_2)_4CH_3$ $\Delta_f H^o(R) = 2$ (8.2)	98.0	410.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

3.2 *Chain unsaturated hydrocarbons*

Table 3.2 C–H BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
acetylene HC≡C–**H** $\Delta_f H^o(R)$ = 135.1±0.7 (565.3±2.9)	(1) 134.9±1.2 (2) 132.9±0.7	564.4±5.0 556.1±2.9	(1) AE (2) Photoelectric detachment	(1) 1979BER (2) 1990ERV/GRO
	(3) 133.1±0.7	556.9±2.9	(3) GPA	(3) 1994BER/ELL
	(3) **132.8±0.7**	**556.6±2.9**	(3) Recommend.	
	(4) 133.3±0.1	557.8±0.3	(4) Photolysis	(4) 1994MOR/ASH
	(5) 131.3±0.7	549.4±2.9	(5) Electron affinity	(5) 2002KIR/TSC
propyne CH_3–C≡C–**H** $\Delta_f H^o(R)$ = 121.0±3.0 (506.3±12.6)	130.2±3.0 at 0K	544.8±12.6 at 0K	Photoelectric spectroscopy	1995ROB/POL
diaicetylene HC≡C–C≡C–**H**	128.8±2.9 at 0K	539.0±12.0 at 0K	Ion beam tandem MS	2000SHI/ERV
propyne CH≡C–CH_2–**H** $\Delta_f H^o(R)$ = 81.0±1.0 (339±4)	(1) 89.2±2.4 (2) 87.2±2 (3) 90.3±3 (4) **88.9±1.0** (5) 91.8±1.0	373.2±10.0 364.8±8.4 377.8±12.6 **372.0±4.2** 384.1±4.2	(1) VLPP (2) AE (3) GPA (4) Recommend. (5) SPST	(1) 1979KIN/NGU (2) 1988HOL/POS (3) 1995ROB/POL (4) 1996TSA (5) 1999TSA
2-butyne CH_3C≡C–CH_2–**H** $\Delta_f H^o(R)$ = 70.2±2 (293.7±8.4)	(1) 90.7 (2) **87.4±2** (3) 84.8	379.5 **365.7±8.4** 354.8	(1) SPST (2) VLPP (3) Correlation	(1) 1978TSA (2) 1982NGU/KIN (3) 2000DEN/DEN
1-butyne HC≡C–C**H**$_2$–CH_3 $\Delta_f H^o(R)$ = 70.5±2.2 (295.0±9.2)	(1) **85.0** (2) 87.3 (3) 83.1±2.2 (4) 82.9	**355.6** 365.3 347.7±9.2 346.8	(1) VLPP (2) SPST (3) Review (4) Correlation	(1) 1981NGU/KIN (2) 1981TSA (3) 1982MCM/GOL (4) 2000DEN/DEN

(continued)

Table 3.2 (continued) C–H BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-penten-3-yne CH_2=CH–C≡C–CH_2–**H** $\Delta_f H^o(R)$ = 84.0 (351.5)	86.8	363.3	VLPP	1992STA/KIN
2-pentyne $CH_3C{\equiv}C{-}C\mathbf{H}_2{-}CH_3$ $\Delta_f H^o(R)$ = 65.2±2.2 (272.8±9.2)	87.3±2.3	365.3±9.6	VLPP	1981KIN/NGU
1-pentyne $HC{\equiv}C{-}C\mathbf{H}_2CH_2CH_3$ $\Delta_f H^o(R)$ = 66.2±2 (277.0±8.4)	83.6±2	349.8±8.4	AE	1976LOS/TRA
3-methyl-1-butyne $HC{\equiv}C{-}C\mathbf{H}(CH_3)_2$ $\Delta_f H^o(R)$ = 61.5±2.2 (257.3±9.2)	(1) **82.5±2** (2) 81.0±2.3	**345.2±8.4** 338.9±9.6	(1) AE (2) VLPP	(1) 1976LOS/TRA (2) 1977KIN
4-methyl-2-pentyne $CH_3C{\equiv}C{-}C\mathbf{H}(CH_3)_2$ $\Delta_f H^o(R)$ = 53.0±2.2 (221.8±9.2)	82.3±2.7	344.3±11.3	VLPP	1981KIN/NGU
5-decyne $CH_3(CH_2)_3C{\equiv}CC\mathbf{H}_2(CH_2)_2CH_3$	83.2	348.0	Correlation	2001TUM/DEN
ethylene H_2C=CH–**H** $\Delta_f H^o(R)$ = 71.6±0.8 (299.6±3.3)	(1) 111.1±2.2 (2) 110.1±2 (3) 110.2±2 (4) **111.2±0.8**	464.8±9.2 460.7±8.4 461.1±8.4 **465.3±3.3**	(1) ICR (2) Kinetics (3) Review (4) Recommend.	(1) 1980DEF/MCI (2) 1981STE/ROW (3) 1982MCM/GOL (4) 1994BER/ELL

	(5) 110.2±0.4	461.1±1.3	(5) FT-IR-GC detection	(5) 1996KAI/WAL
allene CH_2=C=CH–**H** $\Delta_f H^o(R)$ = 81.0±1 (338.9±4)	(1) 92.4±1.2 (2) **88.7±3**	386.6±5.0 **371.1±12.6**	(1) Kinetics (2) GPA	(1) 1971WAL (2) 1995ROB/POL
propene CH_3CH=CH–**H** $\Delta_f H^o(R)$ = 63.8±1.5 (266.9±6)	(1) 109±2.4 (2) **111.1**	456.1±10.0 **464.8**	SPST	(1) 1988CUI/HE (2) 1999TSA
propene CH_2=CH–CH_2–**H** $\Delta_f H^o(R)$ = 40.8±0.7 (171±3)	(1) 86.7±1.5 (2) 87.2±0.5 (3) 88.8±0.4 (4) **88.2±0.7** (5) 87.0±1.1	362.8±6.3 364.8±2.1 371.5±1.7 **368.6±2.9** 364.0±4.6	(1) VLPP (2) Pulse shock tube (3) GPA (4) Recommend. (5) PIMS detection	(1) 1979ROS/KIN (2) 1991ROT/BAU (3) 1996ELL/DAV (4) 1996TSA (5) 1997SEE/SLA
(Z)-2-butene (Z)-CH_3CH=CH–CH_2–**H** $\Delta_f H^o(R)$ = 34.9±2 (146±8)	(1) 89.7 (2) 85.0	375.3 355.8	(1) SPST (2) Correlation	(1) 1999TSA (2) 2000DEN/DEN
(E)-2-butene (E)-CH_3CH=CH–CH_2–**H**	85.3	356.8	Correlation	2000DEN/DEN
1-butene CH_2=CH–CH_2–CH_2–**H** $\Delta_f H^o(R)$ = 46.0 (192.5)	98.1	410.5	Photoelectron spectroscopy	1984SCH/HOU
1-butene CH_2=CH–C**H**$_2$–CH_3	(1) 82.3 (2) 81.5±1.5 (3) 82.6±1.3	344.3 341.0±6.3 345.6±5.4	(1) SPST (2) Pyrolysis (3) Review	(1) 1969TSA (2) 1970TRE (3) 1982MCM/GOL

(continued)

Table 3.2 (continued) C–H BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$\Delta_f H^o(R) = 31.8 \pm 1.5$ (133.1±6.3)	(4) **83.8**	**350.6**	(4) Proton affinity	(4) 1987LIA/AUS
	(5) 83.5	349.2	(5) Correlation	(5) 2001TUM/DEN
isobutene $CH_2=C(CH_3)–CH_2–\mathbf{H}$ $\Delta_f H^o(R) = 30.6 \pm 0.6$ (128.0±2.5)	(1) 86.2±1	360.7±4.2	(1) Pyrolysis	(1) 1977TRE/WRI
	(2) **86.7±0.6**	**362.8±2.5**	(2) Shock tube	(2) 1991ROT/BAU
	(3) 89.1	372.8	(3) SPST	(3) 1999TSA
	(4) 85.5	357.6	(4) Correlation	(4) 2001TUM/DEN
1,3-pentadiene $CH_2 = CHCH = CHCH_2–\mathbf{H}$ $\Delta_f H^o(R) = 49 \pm 3$ (205±12.6)	(1) 79.8±1.0	333.9±4.2	(1) Iodination	(1) 1973ONE/BEN
	(2) 79.7±1.0	333.5±4.2	(2) Pyrolysis	(2) 1980TRE
	(3) **83.0±3**	**347.3±12.6**	(3) Review	(3) 1982MCM/GOL
2,3-pentadiene $CH_3CH=C=CHCH_2–\mathbf{H}$	87.3	365.0	Correlation	2000DEN/DEN
1,4-pentadiene $(CH_2=CH)_2CH–\mathbf{H}$ $\Delta_f H^o(R) = 49.7 \pm 1.0$ (207.9±4.2)	(1) 79.5±1.7	332.6±7.1	(1) Isomerization	(1) 1970EGG/JOL
	(2) 76.4	319.7	(2) Pyrolysis	(2) 1982TRE
	(3) **76.6±1.0**	**320.5±4.2**	(3) PAC	(3) 1991CLA/CUL
	(3) 76.6±1.0	320.5±4.2	(3) AE	
1-pentene $CH_2=CH–C\mathbf{H}_2–CH_2CH_3$ $\Delta_f H^o(R) = 26.2 \pm 2$ (109.6±8.4)	(1) 82.5±2	345.2±8.4	(1) AE	(1) 1976LOS/TRA
	(2) 83.4	348.8	(2) Correlation	(2) 2000DEN/DEN
2-methyl-1-butene $CH_2=C(CH_3)–C\mathbf{H}_2CH_3$	83.0	347.3	Correlation	2000DEN/DEN
3-methyl-1-butene $CH_2=CH–C\mathbf{H}(CH_3)_2$	(1) **79.5±1.7**	**332.6±7.1**	(1) Isomerization	(1) 1970EGG/JOL
	(2) 76.4	319.7	(2) Pyrolysis	(2) 1982TRE

$\Delta_f H^o(R) = 20.8 \pm 2$ (87.0±8.4)	(3) 83.1	347.7	(3) Reanalysis of pyrolysis data	(3) 1998BRO/BEC
	(4) 81.2	339.6	(4) Correlation	(4) 2000DEN/DEN
3-methyl-2-butene $CH_3CH=C(CH_3)CH_2$–**H**	84.2	352.4	Correlation	2000DEN/DEN
2-ethyl-1-propene $CH_2=C(CH_3CH_2)$–CH_2–**H** $\Delta_f H^o(R) = 26.2 \pm 2$ (109.6±8.4)	85.1±2	356.1±8.4	AE	1976LOS/TRA
(E)-2-pentene (E)-$CH_3CH=CHCH_2CH_3$	(1) 81.7±1.5	341.8±6.3	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 82.5	345.2	(2) Correlation	(2) 2000DEN/DEN
(Z)-2-pentene (Z)-$CH_3CH=CHCH_2CH_3$	(1) 80.6±1.5	337.2	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 82.6	345.4	(2) Correlation	(2) 2000DEN/DEN
1-hexene $CH_2=CHCH(CH_2)_2CH_3$	83.4	348.8	Correlation	2001TUM/DEN
3-methyl-1,4-pentadiene $(CH_2=CH)_2C(CH_3)$–**H** $\Delta_f H^o(R) = 46.3$ (202.0)	77	322.2	PAC	1999LAA/MUL
(Z)-4-methyl-2-pentene (Z)-$(CH_3)_2CHCH=CHCH_3$	79.8	333.9	Correlation	2001TUM/DEN
4-methyl-3-pentene $(CH_3)_2C=CHCH_2CH_3$	79.3	331.9	Correlation	2001TUM/DEN

(continued)

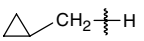
Table 3.2 (continued) C–H BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,3-dimethyl-2-butene $(CH_3)_2C{=}C(CH_3){-}CH_2{-}\mathbf{H}$ $\Delta_f H^o(R) = 9.5\pm1.5$ (39.7 ± 6.3)	(1) 78.0±1.0 (2) 84.7	326.4±4.2 354.3	(1) Iodination (2) Correlation	(1) 1973ROD/WU (2) 2001TUM/DEN
2,3-dimethy-1-butene $CH_2{=}C(CH_3){-}C\mathbf{H}(CH_3)_2$ $\Delta_f H^o(R) = 9\pm1.5$ (37.7 ± 6.3)	(1) 76.3±1.0 (2) 84.3	319.2 352.8	(1) Iodination (2) Correlation	(1) 1973ROD/WU (2) 2001TUM/DEN
(Z)-2,5-dimethyl-3-hexene $(Z)\text{-}(CH_3)_2C\mathbf{H}CH{=}CHCH(CH_3)_2$	80.3	336.1	Correlation	2001TUM/DEN
1,3-octediene $CH_2{=}CHCH{=}CHC\mathbf{H}_2(CH_2)_2CH_3$	79.3	332.0	Correlation	2001TUM/DEN
1-octene $CH_2 = CHC\mathbf{H}_2(CH_2)_4CH_3$	83.4	348.9	Correlation	2000DEN/DEN
(E)-2-octene $(E)\text{-}CH_3CH{=}CHC\mathbf{H}_2(CH_2)_3CH_3$	81.9	342.7	Correlation	2000DEN/DEN
1,8-nonediene $CH_2{=}CHC\mathbf{H}_2(CH_2)_4CH{=}CH_2$	83.6	349.8	Correlation	2001TUM/DEN
Z,Z-2,8-decediene $CH_3CH{=}CH(C\mathbf{H}_2)_4CH{=}CHCH_3$	81.6	341.6	Correlation	2001TUM/DEN
1-hexadecene $CH_2{=}CHC\mathbf{H}_2(CH_2)_{12}CH_3$	83.4	348.8	Correlation	2001TUM/DEN

allyl triphenyl phosphonium bromide $Ph_3P^+C\mathbf{H}_2CH{=}CH_2\ Br^-$	85.9	359.4	AOP	1996ZHA/FRY
3-phenyl-allyl triphenyl phosphonium bromide $Ph_3P^+C\mathbf{H}_2CH{=}CHPh\ Br^-$	81.0	338.9	AOP	1996ZHA/FRY

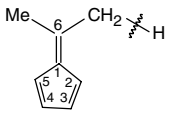
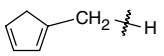
3.3 *Cyclic hydrocarbons*

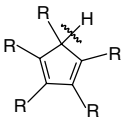
Table 3.3 C–H BDEs in Cyclic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_fH^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
cyclopropene  $\Delta_fH^o(R) = 105.1\pm4.1$ (439.7±17.2)	90.4±4.0	378.3±12.6	ICR	1980DEF/MCI
cyclopropane  $\Delta_fH^o(R) = 66.9\pm0.3$ (279.9±1.3)	(1) 101±3	422.6±12.6	(1) Polanyi correlation	(1) 1966KER
	(2) 100.2±0.4	419.3±1.7	(2) Kinetics	(2) 1978APP/KLU
	(3) **106.3±0.25**	**444.8±1.0**	(3) VLPP	(3) 1979BAG/BEN
	(4) 105.9±2.7	443.1±11.3	(4) ICR	(4) 1980DEF/MCI
	(5) 102.5	429.0	(5) Correlation	(5) 2001TUM/DEN
methylcyclopropane  $\Delta_fH^o(R) = 51.1\pm1.6$ (213.8±6.7)	97.4±1.6	407.5±6.7	Iodination	1971MCM/GOL

(continued)

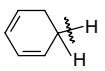
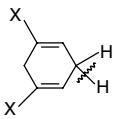
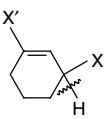
Table 3.3 (continued) C–H BDEs in Cyclic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyclobutane 				
$\Delta_f H^o(R)$ = 51.4±1.0 (215.1±4.2)	(1) 95±3	397.5±12.6	(1) Polanyi correlation	(1) 1966KER
	(2) 96.5	403.8	(2) Polanyi correlation	(2) 1971FER/WHI
	(3) **96.8±1.0**	**405.0±4.2**	(3) Iodination	(3) 1972MCM/GOL
	(4) 97.8±0.3	409.2±1.3	(4) Kinetics	(4) 1978APP/KLU
	(5) 100.0	418.5	(5) Correlation	(5) 2001TUM/DEN
6,6-dimethylfulvene 	84.5	353.5	AOP	1989BOR/HAR
1,3-cyclopentadienes, substituted 	86.5±2	361.9±8.4	VLPP	1981STE
1,3-cyclopentadienes, substituted 	(1) 82.9±2.2	346.9±9.2	(1) ICR	(1) 1980DEF/MCM
	(2) 81.2	339.7	(2) AOP	(2) 1988BOR/CHE
	(3) **83.9±0.5**	**351.0±2.1**	(3) Electrochem.	(3) 1991PAR/HAN
	(4) 81.5±2.7	341.0±11.3	(4) ICR	(4) 1997ROM/JAN
	(5) 82.5±1	345.2±4.2	(5) Reflected shock tube	(5) 2001ROY/BRA
at 1 site H $\Delta_f H^o(R)$ = 63.9±2.0 (267.4±8.4)				
at 1,4 site Ph_2	(6) 75	313.8	(6) AOP	(6) 1991BOR/CHE

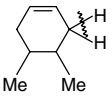
1,3-cyclopentadienes, substituted 				
R = Me $\Delta_f H^o$(pentamethyl-cyclopentadienyl) = 16.1±1.0 (67.4±4.2)	(1) 77	322.2	(1) AOP	(1) 1989BOR/HAR
Ph	(1) **78** (2) 74.1	**326.4** 310.0	(2) Pyrolysis	(2) 1995ROT/HUN
cyclopentene 				
$\Delta_f H^o$(R) = 38.4±1.0 (160.7±4.2)	(1) 82.3±1 (2) 82±2 (3) 81.9	344.3±4.2 343.1±8.4 342.5	(1) Iodination (2) AE (3) Correlation	(1) 1970FUR/GOL(b) (2) 1976LOS/TRA (3) 2000DEN/DEN
cyclopentane, substituted 				
$\Delta_f H^o$(R) = 25.3±1.0 (105.9±4.2) X = H	(1) 94.9±1 (2) 95.0±2 (3) 96.0±0.2 (4) **95.6±1** (5) 97.6	397.1±4.2 397.5±8.4 401.7±0.8 **400.0±4.2** 408.5	(1) Iodination (2) AE (3) Kinetics (4) Radical buffer (5) Correlation	(1) 1970FUR/GOL (2) 1976LOS/TRA (3) 1978APP/KLU (4) 1982CAS/GRI (5) 2001TUM/DEN
Me	(5) 93.7	392.2		
Et	(5) 93.7	392.3		
Ph	(6) 81.9	342.7	(6) Correlation	(6) 1995TUM/DEN
3-tert-butylbicyclo[1.1.1]-pentane 	109.7±3.3	459.0±13.8	GPA	2002REE/KAS

(continued)

Table 3.3 (continued) C–H BDEs in Cyclic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
spiropentane 				
$\Delta_f H^o(R)$ = 91.0±1.0 (380.7±4.2)	98.8±1.0	413.4±4.2	Polanyi correlation	1971FER/WHI
1,3-cyclohexadiene 				
$\Delta_f H^o(R)$ = 47.6 (199.2)	(1) 73±5	305.4	(1) Review	(1) 1982MCM/GOL
	(2) 73.2	306.3	(2) Kinetics	(2) 1985DEA
	(3) **74.3**	**310.9**	(3) VLPP	(3) 1991STE/BRO
	(4) 74.3	310.9	(4) PAC	(4) 1997LAA/MUL
	(5) 79.1	331.1	(5) Correlation	(5) 2001TUM/DEN
1,4-cyclohexadiene, substituted 				
$\Delta_f H^o(R)$ = 48.2±1.2 (201.7±5.0)	(1) 70	292.9	(1) Pyrolysis	(1) 1968JAM/SUA
	(2) **76.0±1.2**	**318.0±5.0**	(2) SPST	(2) 1986TSA
X = H	(3) 73±2	305.4±8.4	(3) PAC	(3) 1989GRI/WAY
	(4) 77	322.2	(4) PAC	(4) 1999CIR/KOR
	(5) 75.0	313.7	(5) Correlation	(5) 2001TUM/DEN
Me	(5) 80.4	336.4		
cyclohexene, substituted 				

$\Delta_f H^o(R)$ = 28.6 (119.7)	(1) 81.9	342.7	(1) AOP	(1) 1988BOR/CHE
X = H X′ = H	(2) 81.6	341.4	(2) Correlation	(2) 2000DEN/DEN
	(3) 81.0	338.9	(3) Correlation	(3) 2001TUM/DEN
Me H	(3) 79.5	332.7		
cyclohexene, substituted	78.0	326.2	Correlation	2001TUM/DEN



cyclohexane, substituted

$\Delta_f H^o(R)$ = 18±1.5 (75.3±6.3)	(1) 96.2	402.5	(1) Kinetics	(1) 1978APP/KLU
X = H	(2) **99.5**	**416.3**	(2) SPST	(2) 1981TSA
	(3) 96.4±0.6	403.3±2.5	(3) EPR	(3) 1982CAS/GRI
	(4) 98	410.0	(4) PAC	(4) 1999CIR/KOR
	(5) 97.6	408.4	(5) Correlation	(5) 2001TUM/DEN
Me	(5) 94.3	394.6		
Et	(5) 94.5	395.4		
$CH=CH_2$	(5) 81.7	341.8		
Ph	(6) 85.2	356.4	(6) Correlation	(6) 2000DEN/DEN

cyclohexane, substituted

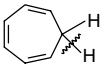
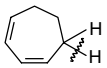
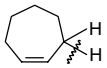
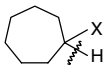
Z 

E 

(Z)-1,2-Me_2	93.9	392.9	Correlation	2001TUM/DEN
(E)-1,2-Me_2	97.4	407.5		
(Z)-1,3-Me_2	93.9	392.9		
(E)-1,3-Me_2	93.2	389.9		
(Z)-1,4-Me_2	93.7	392.0		
(E)-1,4-Me2	94.8	396.6		

(continued)

Table 3.3 (continued) C–H BDEs in Cyclic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1,3,5-cycloheptatriene 				
$\Delta_f H^o(R)$ = 68.2±3 (285.3±12.6)	(1) 82.9±7	346.9±29.3	(1) Electron impact	(1) 1960HAR/HON
	(2) 73±1	305.4±4.2	(2) Pyrolysis	(2) 1969VIN/DAU
	(3) 73±2	305.4±8.4	(3) ICR	(3) 1979BAR/SCO
	(4) **76.6±3**	**320.5±12.6**	(4) ICR	(4) 1980DEF/MCM
	(5) 73.2±2	306.3±8.4	(5) Review	(5) 1982MCM/GOL
1,3-cycloheptadiene 	83.0	347.3	Correlation	2001TUM/DEN
cycloheptene 	82.9	346.9	Correlation	2001TUM/DEN
cycloheptane, substituted 				
$\Delta_f H^o(R)$ = 12.1±1.0 (50.6±4.2)				
X = H	(1) 93.3	389.1±12.6	(1) Polanyi correlation	(1) 1966KER
	(2) **94.0**	**393.3**	(2) Kinetics	(2) 1970JON/WHI
	(3) 92.5±1	387.0±4.2	(3) Photobromin.	(3) 1971FER/WHI
	(4) 92.5±1	387.0±4.2	(4) Review	(4) 1982MCM/GOL
	(5) 96.5	403.8		
Me	(5) 93.0	389.0	(5) Correlation	(5) 2001TUM/DEN
Et	(5) 93.8	392.4		

norbornene

$\Delta_f H^o(R)$ = 32.6±2.5 (136.4±10.5)	(1) **96.7±2.5** (2) 99.4	**404.6±10.5** 415.9	Iodination	(1) 1970ONE/BAG (2) 1971DAN/TIP

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quadricyclane

$\Delta_f H^o(R)$ = 138.3±1.3 (578.6±5.4)	109.4±1.3	457.7±5.4	Ion flow tube	1996LEE/DEP

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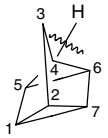
quadricyclane



$\Delta_f H^o(R)$ = 140.4±1.3 (587.4±5.4)	111.5±1.3	466.5±5.4	Ion flow tube	1996LEE/DEP

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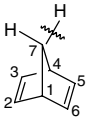
norboradine



$\Delta_f H^o(R)$ = 122.3±1.9 (511.7±7.9)	115.6±1.9	483.7±7.9	Ion flow tube	1996LEE/DEP

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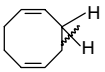
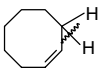
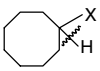
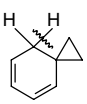
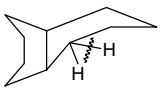
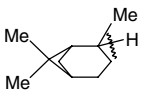
cubane

$\Delta_f H^o(R)$ = 198.6±4 (830.9±16.7)	102±4	426.8±16.7	GPA	1997HAR/EMR

(continued)

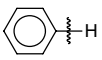
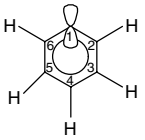
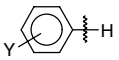
Table 3.3 (continued) C–H BDEs in Cyclic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
bicyclooctane 				
$\Delta_f H^o(R)$ = 22.0 (92.0)	97.7	408.8	Kinetics	1971DAN/TIP
cyclooctadiene 	79.3	331.8	Correlation	2001TUM/DEN
cyclooctene 	85.4	357.2	Correlation	2001TUM/DEN
cyclooctane, substituted 				
X = H	95.7	400.2	Correlation	2001TUM/DEN
Me	94.4	395.0		
Et	93.7	392.2		
spiro[2.5]-octa-4,6-diene 	70.7	295.6	Correlation	2001TUM/DEN
cyclononane cyclo-C_9H_{17}–**H**	96.3	403.9	Correlation	2001TUM/DEN

adamantane 				
$\Delta_f H^o$(R, at 1 site) = 12.3 (51.5)	(1) 97.0 (2) 96.2 (3) 98.5 (4) 93.0	405.8 402.5 412.0	(1) Kinetics (2) AP (3) Correlation (4) Derived	(1) 1971DAN/TIP (2) 1998AUB/HOL (3) 2001TUM/DEN (4) 2001MAT/LEB
$\Delta_f H^o$(R, at 2 site) = 14.8 (61.9)	(2) 100.2 (3) 98.5 (3) 98.4	419.2 412.0 411.7	(5) Photoelectr. spectroscopy	(5) 1986KRU/BEA
cyclodecane cyclo-$C_{10}H_{19}$–**H**	96.7	404.5	Correlation	2001TUM/DEN
cycloundecane cyclo-$C_{11}H_{21}$–**H**	96.7	404.7	Correlation	2001TUM/DEN
cyclododecane cyclo-$C_{12}H_{23}$–**H**	98.0	410.0	Correlation	2001TUM/DEN
(Z)-decalin 	93.5	391.1	Correlation	2001TUM/DEN
(E)-decalin 	95.6	400.0	Correlation	2001TUM/DEN
(Z)-pinane 	90.2	377.4	Correlation	2001TUM/DEN

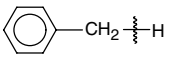
3.4 *Aromatic hydrocarbons*

Table 3.4 C–H BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
benzene 				
$\Delta_f H^o(R)$ = 78.9±0.8 (330.1±3.3)	(1) 112.3±1	469.9±4.2	(1) Iodination	(1) 1967ROD/GOL
	(2) 111.2±0.8	465.3±3.3	(2) GPA, recommend.	(2) 1994BER/ELL
	(3) 113.5±0.5	474.9±2.1	(3) Ion flow tube	(3) 1995DAV/BIE
	(4) 113.3±2	474±8	(4) Recommend.	(4) 1996TSA
	(5) **112.9±0.5**	**472.2±2.2**	(5) GPA, revised	(5) 2002ERV/DET
phenyl 				
C–H at site 2	79.9±3.1	334.3	CID	1994WEN/SQU
3	95.3±3.2	398.7		
4	110.6±3.4	462.8±14.2		
benzene, substituted 				
Y = 2-C(O)O$^-$	113.9	476.6	Correlation	1998NAS/SQU
3-C(O)O$^-$	110.4	461.9		
4-C(O)O$^-$	112.3	469.9		
2-C(O)OH $\Delta_f H^o(R)$ = –7.9 (–33.1)	114.5	479.1		
3-C(O)OH $\Delta_f H^o(R)$ = –8.4 (–35.1)	114.0	477.0		

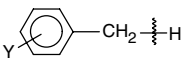
4-C(O)OH	113.8	476.1		
$\Delta_f H^o(R) = -8.6\ (-36.0)$				

toluene



$\Delta_f H^o(R) = 48.4 \pm 1.5$	(1) 87.9±1.5	367.8±6.3	(1) VLPP	(1) 1979ROS/GOL
(202.5±6.3)	(2) 88.1±2.2	368.6±9.2	(2) ICR	(2) 1980DEF/MCI
	(3) 88.6	370.7	(3) SPST	(3) 1990WAI/TSA
	(4) **88.5±1.5**	**370.3±6.3**	(4) Recommend.	(4) 1994BER/ELL
	(5) 89.6±1.0	375±4	(5) Recommend.	(5) 1996TSA

toluene, substituted



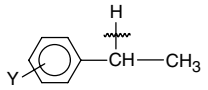
Y = 3-F	(2) 89.3	373.6	(1) Photoelectr. spectroscopy	(1) 1986HAY/KRU
4-F	(2) 89.7	375.1	(2) Correlation	(2) 2000DEN/DEN
3-Cl	(2) 89.1	373.0		
4-Cl	(2) 88.7	371.3		
3-Br	(2) 89.7	375.4		
4-Br	(3) 90.8	380.1	(3) Correlation	(3) 2002KRO/TUM
2-CH_3	(1) 87.3	365.3		
	(2) 89.6	375.0		
3-CH_3	(1) 87.8	367.4		
	(2) 88.8	371.4		
4-CH_3	(1) 87.7	366.9		
	(2) 88.4	369.7		
4-Et	(3) 87.0	363.9		
2-Pr	(3) 87.6	366.6		
3-Pr	(3) 86.8	363.2		
4-Pr	(3) 87.0	363.9		
4-tBu	(2) 89.4	374.1		
3-CN	(3) 88.7	371.0		
4-CN	(3) 88.0	368.0		

(continued)

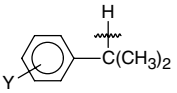
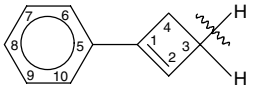
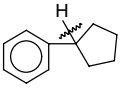
Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
3-NO_2	(3) 89.6	375.0		
4-NO_2	(2) 89.2 (4) 86.5	373.4 361.9	(4) AOP	(4) 1995BOR/ZHA(c)
4-PhO	(2) 89.7	375.4		
4-$PhSO_2$	(5) 88	368.2	(5) AOP	(5) 1993ZHA/BOR
4-CH_2OCH_3	(3) 85.4	357.5		
3-MeO	(3) 90.5	378.8		
4-MeO	(3) 86.6	362.5		
3-EtOC(O)	(3) 89.1	372.7		
4-EtOC(O)	(3) 89.4	374.1		
2,4-Cl_2	(3) 88.6	370.9		
3,4-Cl_2	(2) 88.3	369.6		
2,3-Me_2	(3) 89.5	374.3		
2,4-Me_2	(2) 89.1	373.0		
3,5-Me_2	(2) 89.5	374.3		
2,3,4,5,6-Me_5	(2) 88.6	370.9		
3-CH_2	(6) 90.7±2.9	379.5±12.1	(6) CID	(6) 2000HAM/WEN
3,5-(CH_2·)	(7) 88.2±5.0	369.0±20.9	(7) CID	(7) 2001HAM/WEN

ethylbenzene, substituted

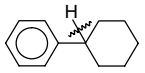


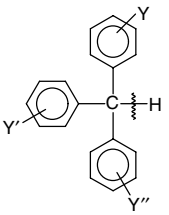
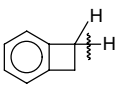
$\Delta_f H^o(R)$ = 40.4 (169.0)	(1) 84.6	354.0	(1) VLPP	(1) 1981ROB/STE
	(2) 86.2	360.7	(2) Proton affinity	(2) 1982MEO
Y = H	(3) **85.4±1.5**	**357.3±6.3**	(3) Review	(3) 1982MCM/DOL
	(4) 90.3	377.8	(4) Reanal. of pyrolysis data	(4) 1998BRO/BEC
	(5) 87.0	364.1		(5) 2000DEN/DEN

p-C_2H_5	(6) 86.3	361.1	(6) Correlation	(6) 2002KRO/TUM
p-Br	(6) 87.1	364.4	(6) Correlation	
p-tBu	(6) 86.5	361.9		
p-MeOC(O)	(6) 87.0	364.1		
prop-2-enylbenzene Ph$C\mathbf{H}_2CH{=}CH_2$	84.4	353.1	Correlation	1995TUM/DEN
n-propylbenzene Ph$C\mathbf{H}_2C_2H_5$	(1) 86.1 (2) 87.5	360.2 366.2	(1) Proton affinity (2) Correlation	(1) 1982MEO (2) 2000DEN/DEN
i-propylbenzene, substituted  				
Y = 2,5-Me_2	86.7	362.8	Correlation	2002KRO/TUM
4-t-Bu	83.5	349.3		
t-butylbenzene $C_6H_5C(CH_3)_2CH_2$–**H**	98.7	413.0	Correlation	2002KRO/TUM
(E)-1-phenylpropene (E)-Ph-CH=CH-CH_2–**H**	78.9±2.6	330.1±10.9	FT-MS	2002GLA/MAK
1-phenylcyclobutene  	85.6±2.6	358.2±10.9	FT-MS	2002GLA/MAK
cyclopentylbenzene  	88.0	268.2	Correlation	2002KRO/TUM

(continued)

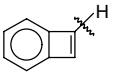
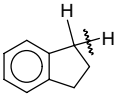
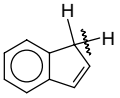
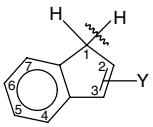
Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyclohexylbenzene 	85.2	356.4	Correlation	2002KRO/TUM
diphenylmethane $Ph_2C\mathbf{H}_2$ $\Delta_f H^o(R)$ = 72.2±1.0 (302.1±4.2)	(1) 84±2 (2) 82 (3) **84.5±0.5** (4) 85.8 (5) 85.3	351.5±8.4 343.1 **353.5±2.1** 359.0 356.9	(1) VLPP (2) AOP (3) Electrochem. (4) Reanal. of pyrolysis data (5) Correlation	(1) 1991STE/BRO (2) 1991BOR/CHE (3) 1991PAR/HAN (4) 1998BRO/BEC (5) 2000DEN/DEN
diphenylmethane, substituted $(p\text{-}PhC_6H_4)_2C\mathbf{H}_2$	80	334.7	AOP	1989BOR/HAR
1,2-diphenylethane $PhC\mathbf{H}_2CH_2Ph$	87.0	364.1	Correlation	2000DEN/DEN
2-phenylpropane $Ph(CH_3)_2C$–**H** $\Delta_f H^o(R)$ = 32.0±1.0 (133.9±4.2)	(1) 83.6 (2) 84.4±1.5 (3) **83.2±1** (4) 87.3 (5) 84.8	349.8 353.1±6.3 **348.1±4.2** 365.3 354.7	(1) VLPP (2) Review (3) PAC (4) Reanal. of pyrolysis data (5) Correlation	(1) 1981ROB/STE (2) 1982MCM/GOL (3) 1997LAA/BOR (4) 1998BRO/BEC (5) 2000DEN/DEN
1,1-diphenylethane $Ph_2C(CH_3)C$–**H**	(1) 81±2 (2) **82.8** (3) 83.9	338.9±8.4 **346.4** 351.0	(1) VLPP (2) Reanal. of pyrolysis data (3) Correlation	(1) 1981STE (2) 1998BRO/BEC (3) 2000DEN/DEN

thiphenylmethane, substituted 					
$\Delta_f H^o(Ph_3C)$ = 93.7±2.0		(1) **81±2**	**338.9±8.4**	(1) AOP	(1) 1991PAR/HAN
(392.0±8.4)		(2) 80.8±3	338.1±12.6	(2) AOP	(2) 1993BOR/ZHA(b)
Y = p-H Y′ = p-H Y″ = p-H		(3) 79.0	330.5	(3) AOP	(3) 1997ARN/FLO
		(4) 82.7	346.0	(4) Correlation	(4) 2000DEN/DEN
		(5) 85.4	357.3	(5) Correlation	(5) 2002KRO/TUM
Y = p-MeO	p-MeO p-MeO	(3) 78.1	326.8		
p-MeO	p-MeO p–H	(3) 79.3	331.8		
p-Me	p-Me p-Me	(3) 79.0	330.5		
p-MeO	p–H p–H	(3) 80.7	337.6		
p-Me	p-Me p–H	(3) 80.3	336.0		
p-Me	p–H p–H	(3) 79.1	331.0		
p-tBu	p-tBu p-tBu	(3) 74.4	311.3		
thiphenylmethane, substituted $(p–HC_6F_4)_3C–$**H**		82.3	344.3	AOP	1993BOR/ZHA(b)
1,1,3,3-tetraphenylpropene $Ph_2C=CHC(Ph)_2$**H**		77	322.2	AOP	1989BOR/HAR
1,1,3,5,5-pentaphenyl-1,4-pentadiene $Ph_2C=CHC$**H**$(Ph)CH=CPh_2$		75.1	314.2	AOP	1991BOR/CHE
benzocyclobutene 		92±4	384.9±16.7	FT-MS	2000GLA/MAK

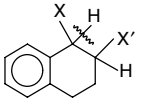
(continued)

Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
benzocyclobutadiene 	114±4	477.0±16.7	FT-MS	2000BRO/KAS(b)
indane 				
$\Delta_f H^o$(indanyl) = 48.8±2.0 (204.2±8.4)	85.9	359.4	Correlation	2000DEN/DEN
indene 				
$\Delta_f H^o$(indenyl) = 71 (297.1)	(1) 84±3	351.5±12.6	(1) Review	(1) 1982MCM/GOL
	(2) 81.5±0.5	341.0±2.1	(2) Electrochem.	(2) 1991PAR/HAN
	(3) 81.1±2.4	339.3±10.0	(3) ICR	(3) 1997ROM/JAN
	(4) **83.0**	**347.3**	(4) Reanal. of pyrolysis data	(4) 1998BRO/BEC
	(5) 81.2	339.7	(5) Correlation	(5) 2001TUM/DEN
indene, substituted 				
Y = 2-Br	(1) 80.9	338.5	(1) AOP	(1) 1992BOR/SAT
3-Me	(1) 77.6	324.7		
3-t-Bu	(1) 78.5	328.4		
2-Ph	(1) 79.3	331.8		
	(2) 84±3	351.5±12.6	(2) VLPP	(2) 1981STE

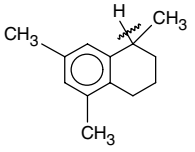
3-Ph	(1) 75.3	315.1		
3-MeO	(1) 76.4	319.7		
3-MeS	(1) 74.1	310.0		
2-PhS	(1) 80.2	335.6		
3-CN	(1) 77.9	325.9		
3-c-C_4H_8N	(1) 70.3	294.1		
2-c-C_4H_8N	(1) 83.5	349.4		
3-c-$C_5H_{10}N$	(1) 72.3	302.5		
2-c-$C_5H_{10}N$	(1) 82.5	345.2		
3-c-OC_4H_8N	(1) 73.4	307.1		
2-c-OC_4H_8N	(1) 82.8	346.4		
2-(4-$MeOC_6H_4$)	(1) 79.3	331.8		
2-(4-MeC_6H_4)	(1) 79.1	331.0		
3-$C(O)NH_2$	(1) 77.7	322.2		
2-C(O)OMe	(1) 79.2	331.4		
3-C(O)OMe	(1) 77.6	324.7		
6-NO_2–3-Me	(1) 78.4	328.0		
1,2,3-Ph_3	(1) 75.8	317.1		

tetralin



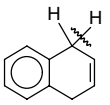
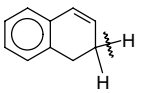
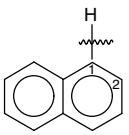
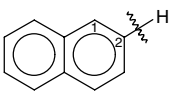
Δ_fH^o(R) = 37±1.2	(1) 82.9±1.2	346.9±5.0	(1) PAC	(1) 1997LAA/MUL
(154.8±5.0)	(2) 83.6	349.6	(2) Correlation	(2) 2000DEN/DEN
X = H X′ = H	(3) 82.6	345.6	(3) Correlation	(3) 2002KRO/TUM
Me H	(4) 79.3	331.8	(4) Correlation	(4) 1995TUM/DEN
	(3) 80.4	336.4		
Me Me	(4) 80.5	336.8		

1,5,7-trimethyltetralin	80.9	338.4	Correlation	2002KRO/TUM

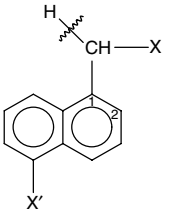


(continued)

Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

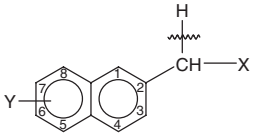
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1,4-dihydronaphthalene 	83.0	347.3	Reanal. of pyrolysis data	1997RUC/GER
1,2-dihydronaphthalene 	(1) 86.0	359.8	(1) Reanal. of pyrolysis data	(1) 1997RUC/GER
	(2) 80.4	336.4	(2) Correlation	(2) 2002KRO/TUM
naphthalene 				
$\Delta_f H^o(R)$ = 96.0±1.3 (401.7±5.4)	(1) **112.2±1.3**	**469.4±5.4**	(1) FT MS	(1) 2000REE/KAS
	(2) 113.4±5.2	474.5±21.8	(2) Negative ion cycle	(2) 2001LAR/SQU
	(3) 112.8±3.3	472.0±14.0	(3) Negative ion spectroscopy	(3) 2001ERV/RAM
naphthalene 				
$\Delta_f H^o(R)$ = 95.7±1.4 (400.4±5.9)	(1) **111.9±1.4**	**468.2±5.9**	(1) FT MS	(1) 2000REE/KAS
	(2) 115.4±4.9	482.8±20.5	(2) Negative ion cycle	(2) 2001LAR/SQU
	(3) 113.8±4.8	476.0±20	(3) Negative ion spectroscopy	(3) 2001ERV/RAM

1-methyl-naphthalene



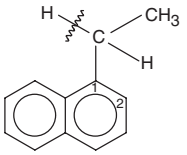
$\Delta_f H^o$(1-naphthylmethyl) = 60.4 (252.7)		(1) 84.3±1.5 (2) **85.1±1.5**	352.7±6.3 **356.1±6.3**	(1) VLPP (2) Review	(1) 1980MCM/TRE (2) 1982MCM/GOL
X = H	X′ = H	(3) 87.3	365.1	(3) Correlation	(3) 2000DEN/DEN
CN	H	(4) 81.3	340.2	(4) AOP	(4) 1988BOR/CHE(b)
H	Me	(5) 86.8	363.3	(5) Correlation	(5) 2002KRO/TUM

2-methyl-naphthalene

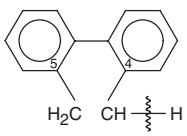


X = H	Y = H	(1) 85.6	358.3	(1) Correlation	(1) 2002KRO/TUM
Me	H	(1) 87.1	364.6		
SO_2Ph	H	(2) 89	372.4	(2) AOP	(2) 1988BOR/BAU
CN	H	(3) 81.4	340.6	(3) AOP	(3) 1988BOR/CHE(b)
H	3-Me	(1) 86.8	363.1		
H	6-Me	(1) 87.3	365.2		

1-ethylnaphthalene	87.1	364.4	Correlation	2000DEN/DEN

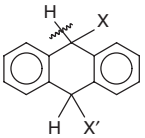
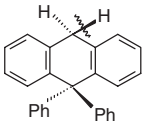
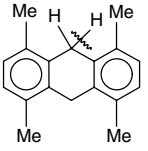


4,5-methylene-phenathrene	81	338.9	AOP	1989BOR/HAR

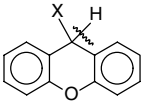


(continued)

Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

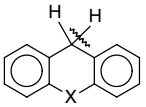
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
9,10-dihydroanthracene, substituted 				
$\Delta_f H^o$(9,10-dihydroanthracen-9-yl) = 62.4 (261.1) X = H, X′ = H	(1) 78 (2) 78 (3) 77 (4) **76.3** (5) 83.0	326.4 326.4 322.2 **319.2** 347.3	(1) AOP (2) PAC (3) Kinetics (4) VLPP (5) Reanal. of pyrolysis data	(1) 1988BOR/CHE (2) 1989GRI/SIM (3) 1990MAL/MCM (4) 1991STE/BRO (5) 1997RUC/GER
H Ph	(6) 79 (5) 84.5	330.5 353.5	(6) AOP	(6) 1991BOR/CHE
Me Me	(7) 77 (5) 81.5	322.2 341.0	(7) PAC	(7) 1989GRI/SIM
9,10-dihydroanthracene, substituted 	84.9	355.2	Reanal. of pyrolysis data	1997RUC/GER
9,10-dihydroanthracene, substituted 	83.3	348.5	Reanal. of pyrolysis data	1997RUC/GER

xanthece, substituted



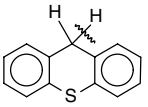
X = H	(1) 74	309.6	(1) VLPP	(1) 1991STE/BRO
	(2) 75.5	315.9	(2) AOP	(2) 1991BOR/CHE
	(3) 75.2	314.6	(3) AOP	(3) 1997ARN/FLO
	(4) 80.7	337.6	(4) Reanal. of pyrolysis data	(4) 1997RUC/GER
Me	(4) 77.6	324.7		
CN	(5) 69	288.7	(5) AOP	(5) 1992ZHA/BOR
SO_2Ph	(6) 82	343.1	(6) AOP	(6) 1988BOR/CHE
Ph	(5) 76	318.0	(7) AOP	(7) 1993ARN/FLO
	(3) 74.6	312.1		
	(7) 76.7	320.9		
p-MeC_6H_4	(5) 75.6	316.3		
p-$MeOC_6H_4$	(5) 74.3	310.9		
	(7) 76.2	318.8		
p-FC_6H_4	(5) 76.8	321.3		
	(7) 76.4	319.7		
p-ClC_6H_4	(5) 73.9	309.2		
	(7) 78.1	326.8		
p-$CF_3C_6H_4$	(5) 78.3	327.6		
	(7) 78.1	326.8		

9,10-dihydroacridine, substituted



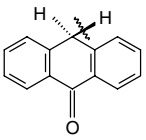
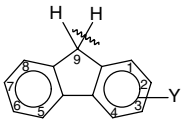
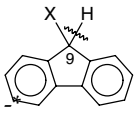
X = NH	80.0	334.8	Reanal. of pyrolysis data	1997RUC/GER
NCH_3	80.0	334.8		

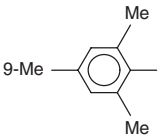
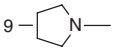
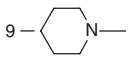
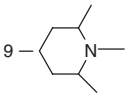
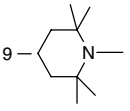
thioxanthece	74.6	312.1	AOP	1997ARN/FLO



(continued)

Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

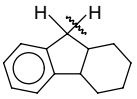
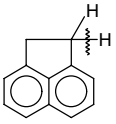
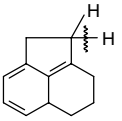
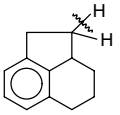
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
10-hydroanthracen-9-one 	80.2	335.6	Reanal. of pyrolysis data	1997RUC/GER
fluorene, substituted 				
$\Delta_f H^o$(9-fluorenyl) = 71.7±2.0 (300.0±8.4)	(1) 80.1	335.1	(1) VLPP	(1) 1991STE/BRO
	(2) 82.2	343.9	(2) Electrochem.	(2) 1992PAR
Y = H	(3) 81.2±2.4	339.7±10.0	(3) ICR	(3) 1997ROM/JAN
	(4) **82.0±2**	**343.1±8.4**	(4) Reanal. of pyrolysis data	(4) 1994RAK/VER
	(5) 82.6	345.6	(5) Reanal. of pyrolysis data	(5) 1997RUC/GER
2-$PhSO_2$	(6) 80	334.7	(6) AOP	(6) 1992ZHA/BOR
2-CN	(6) 80	334.7		
2-NO_2	(6) 81	338.9		
2-MeO	(7) 80	334.7	(7) AOP	(7) 1994ZHA/BOR(b)
2-Me_2N	(6) 80	334.7		
2-$PhSO_2$	(8) 79.7	333.5	(8) AOP	(8) 1993ZHA/BOR
2,7-Br_2-9-CO_2Me	(6) 76.5	320.1		
fluorene, substituted 				
X = 9-CN	(1) 74.8	313.0	AOP	(1) 1991BOR/ZHA

9-SO_2Ph	(1) 81.9	342.7	
9-PhS	(1) 74.6	312.1	
9-Me_2N	(1) 71.5	299.2	
9-(2,4,6-$Me_3C_6H_2$)	(2) 74.5	311.7	(2) 1991BOR/ZHA
9-$PhCH_2$(Me)N	(3) 72.5	303.3	(3) 1992ZHA/BOR
9-$(iPr)_2$N	(3) 73	305.4	
	(3) 76	318.0	
	(3) 68	284.5	
	(3) 72	301.2	
	(3) 72	301.2	
	(3) 71	297.1	
9-Ph	(6) 74	309.6	
9-C_6F_5	(4) 78.2	327.2	(4) 1993ZHA/BOR
9-mesityl	(6) 74.5	311.7	(5) 1994ZHA/BOR(b)
9-MeOCO	(6) 76	318.0	(6) 1994ZHA/BOR(c)
9-c-C_4H_8N	(6) 68	284.5	
9-c-$C_5H_{10}N$	(6) 72	301.2	
9-PhCH(Me)N	(6) 72.5	303.3	
9-$\overline{CH(Me)(CH_2)_2C(Me)NH}$	(6) 72	301.2	
9-$\overline{C(Me)_2(CH_2)_2C(Me)_2N}$	(6) 71	297.1	
9-Me	(7) 75.4	315.5	(7) 1994BOR/ZHA
$\Delta_fH^o(R)$ = 64.1±2	(8) 79.7±2	333.5	(8) 1998BRO/BEC
(268.2±8.4)	(9) 78.5	328.4	(9) 2002KRO/TUM

(continued)

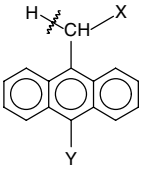
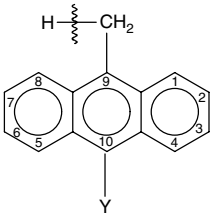
Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
9-Et	(7) 76.2	318.8		
9-n-Pr	(7) 76.1	318.4		
9-iPr	(7) 77.3	323.4		
9-sBu	(7) 75.1	314.2		
9-tBu	(7) 79.9	334.3		
9-neoC_5H_{11}	(7) 73.6	307.9		
9-PhC$(Me)_2CH_2$	(7) 73.8	308.8		
9-PhCH_2	(7) 75.9	317.6		
9-MeS	(7) 74.6	312.1		
9-EtS	(7) 74.3	310.9		
9-iPrS	(7) 74.3	310.9		
9-tBuS	(7) 74.8	313.0		
9-PhS	(7) 74.8	313.0		
9-MeSO_2	(7) 82.1	343.5		
9-EtSO_2	(7) 81.4	340.6		
9-iPrSO_2	(7) 81.1	339.3		
9-PhSO_2	(7) 79.7	333.5		
9-(p-BrPh)SO_2	(7) 82	343.1		
9-MeO	(7) 73.0	305.4		
9-EtO	(7) 72.9	305.0		
9-iPrO	(7) 72.7	304.2		
9-tBuO	(7) 74.0	309.6		
9-PhO	(7) 74.3	310.9		
9-Me_3SiCH_2	(9) 76.3	319.2		(9) 1996ZHA/BOR
9-Me_3N^+, Cl^-	(5) 84.6	354.0		
9-PyN^+, Br^-	(4) 80.9	338.5		

9-Ph_3P^+, Br^-	(5) 81.6	341.4		
9-nBu_3P^+, Br^-	(10) 83.0	347.3		(10) 2000CHE/LIU
9-Ph_3As^+, Br^-	(10) 82.6	345.6		
9-Me_2S^+, Br^-	(10) 77.6	324.7		
9-Me_2Se^+, Br^-	(10) 78.7	329.3		
9-tBu_2Te^+, Br^-	(10) 77.3	323.4		
9-Me_3N^+(2-$PhSO_2$), Br^-	(4) 85.7	358.6		
1,2,3,4,4a, 9a-hexahydrofluorene 	79.3	332.0	Correlation	2002KRO/TUM
acenaphthene 	83.7	350.0	Correlation	2000DEN/DEN
3,4,5-trihydroacenaphthene 	78.8	329.7	Correlation	1995STUM/DEN
tetrahydroacenaphthene 	75.8	317.0	Correlation	2002KRO/TUM

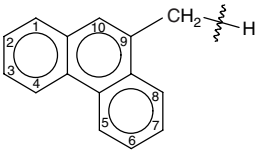
(continued)

Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

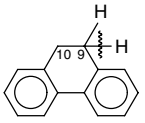
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
9-anthracenylmethane, substituted 				
Y = H, X = H $\Delta_f H^o$(9-anthracenylmethyl) = 80.7 (337.6)	(1) 81.0	338.9	(1) Analysis of exp.	(1) 1980MCM/TRE
	(2) 81.8	342.3	(2) Review	(2) 1982MCM/GOL
	(3) 81.5	341.0	(3) AOP	(3) 1991BOR/CHE
	(4) **84.1±0.5**	**351.9±2.1**	(4) Electrochem.	(4) 1991PAR/HAN
CN	(5) 78.7	329.3	(5) AOP	(5) 1991BAU/FAS(b)
	(6) 78.9	330.1	(6) AOP	(6) 1993ZHA/BOR(b)
MeO	(5) 77.4	323.8		
	(6) 77.5	324.3		
PhO	(5) 78.6	328.7		
	(6) 79.9	334.3		
PhCO	(6) 84.2	352.3		
NO_2	(6) 86.1	360.2		
PhS	(6) 81.0	338.9		
$PhSO_2$	(6) 84.7	354.4		
Y = CN, X = MeO	(5) 73.7	308.4		
PhO	(5) 72.9	305.0		
anthracene, substituted 				
Y = Cl	(1) 80.8	338.1	(1) AOP	(1) 1993ZHA/BOR(b)
Me	(1) 81.8	342.3	(2) Correlation	(2) 2002KRO/TUM
	(2) 78.1	326.7		

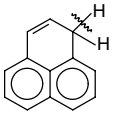
MeO	(1) 81.4	340.6		
Ph	(1) 81.8	342.3		
CHO	(1) 80.4	336.4		
PhCO	(1) 82.3	344.3		
CN	(1) 80	334.7		
NO_2	(1) 82.6	345.6		
PhS	(1) 80.8	338.1		

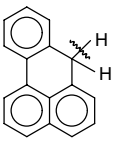
9-phenanthrenylmethane



$\Delta_f H^o$(9-phenanthrenylmethyl) = 74.4 (311.3)	85.1±1.5	356.1±6.5	VLPP	1982MCM/GOL

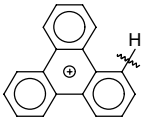
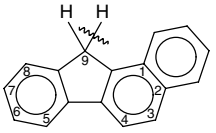
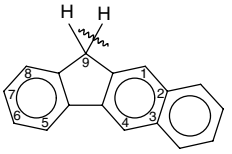
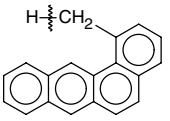
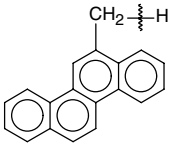
9,10-dihydrophenanthrene	(1) 89.6	374.9	(1) Reanal. of pyrolysis data	(1) 1997RUC/GER
	(2) 82.1	343.7	(2) Correlation	(2) 2000DEN/DEN
	(3) 81.6	341.6	(3) Correlation	(3) 2002KRO/TUM

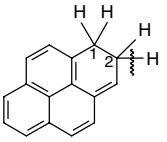
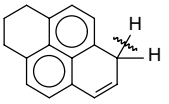
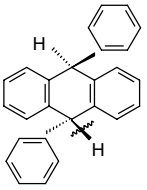
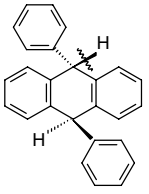
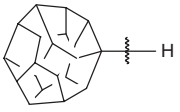
phenalene	(1) 64±3	267.8±12.6	(1) AOP	(1) 1990BAU/GOS
	(2) 74.0	309.6	(2) Reanal. of pyrolysis data	(2) 1997RUC/GER

benzanthrene	(1) 66±3	276.1±12.6	(1) AOP	(1) 1990BAU/GOS
	(2) 76.0	318.0	(2) Reanal. of pyrolysis data	(2) 1997RUC/GER

(continued)

Table 3.4 (continued) C–H BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
triphenylene radical cation 	86.0±4.8	359.9±20.0	PIMS	1997LIN/LIF
1,2-benzofluorence 	78.7	329.3	AOP	1991BOR/CHE
2,3-benzofluorence 	(1) 78.8 (2) 78.4	329.7 328.0	(1) VLPP (2) AOP	(1) 1991STE/BRO (2) 1991BOR/CHE
methylbenzo(b)phenanthrene 	88.6	370.8	Correlation	2002KRO/TUM
6-methylchrysene 	85.7	358.7	Correlation	2002KRO/TUM

1,2-dihydropyrene 	81.6	341.4	Correlation	2000DEN/DEN
1,2,3,6-tetrahydropyrene 	81.6	341.4	Correlation	2002KRO/TUM
(E)-9,10-diphenyl-9, 10-dihydroanthracene 	81.5	341.0	Reanal. of pyrolysis data	1997RUC/GER
(Z)-9,10-diphenyl-9, 10-dihydroanthracene 	79.4	332.2	Reanal. of pyrolysis data	1997RUC/GER
dodecahedrane 	92±3	384.9±12.6	FT-MS	2000BRO/KAS(a)

3.5 *Halogenated hydrocarbons*

Table 3.5 C–H BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
trifluoromethane	(1) 106.7±1	446.4±4.2	(1) Photolysis	(1) 1972BAS/WHI
CF_3–**H**	(2) 107	447.7	(2) Review	(2) 1982MCM/GOL
$\Delta_f H^o(R)$ = –111.4±0.9	(3) **107.4**	**449.4**	(3) Derived	(3) 1997ASH/RUS
(–466.1±3.8)	(4) 106.3±1.3	444.8±5.4	(4) Recommend.	(4) 1998CHA
	(5) 108.9	455.6	(5) SPST	(5) 1999TSA
difluoromethane	(1) 97.4±1.3	407.5±5.4	(1) Kinetics	(1) 1969PRI/PER
CHF_2–**H**	(2) 101±2	422.6±8.4	(2) Elimination	(2) 1971KER/TIM
$\Delta_f H^o(R)$ = –57.1±1	(3) **103.2±1**	**431.8±4.2**	(3) Iodination	(3) 1983PIC/ROD
(–238.9±4.2)	(4) 101±2	422.6±8.4	(4) Kinetics	(4) 1983MAR/PAR
	(5) 101.8±1.1	425.8±4.6	(5) Review	(5) 2001LAZ/PRO
fluoromethane	(1) **101.3±1**	**423.8±4.2**	(1) Iodination	(1) 1983PIC/ROD
CH_2F–**H**	(2) 100±2	418.4±8.4	(2) Kinetics	(2) 1983MAR/PAR
$\Delta_f H^o(R)$ = –7.6±1				
(–31.8±4.2)				
chlorodifluoromethane	(1) 101.6±1	425.1±4.2	(1) Review	(1) 1982MCM/GOL
$CClF_2$–**H**	(2) **100.7±2**	**421.7±8.4**	(2) Photobromin.	(2) 1992MIY/TSC
$\Delta_f H^o(R)$ = –66.7±2				
(–279.1±8.4)				
dichlorofluoromethane	(1) 98.9±1.2	413.8±5.0	(1) Bromination	(1) 1987TSC/PAD
CCl_2F–**H**	(2) **98.2±2**	**410.9±8.4**	(2) Photobromin.	(2) 1992MIY/TSC
$\Delta_f H^o(R)$ = –21.3±2	(3) 97.7	408.8	(3) Review	(3) 1997POU/PAU
(–89.0±8.4)				
chlorofluoromethane	(1) **100.8±2.4**	**421.7±10.0**	(1) Bromination	(1) 1987TSC/PAD
CHClF–**H**	(2) 99.4	415.9	(2) Review	(2) 1997POU/PAU
$\Delta_f H^o(R)$ = –14.5±2.4				
(–60.7±10.0)				

trichloromethane CCl_3–**H** $\Delta_f H^o(R)$ = 17.0±0.6 (71.1±2.5)	(1) 95.8±1 (2) 95.2 (3) 94.9±2 (4) **93.8±0.6**	400.8±4.2 398.3 397.1±8.4 **392.5±2.5**	(1) Bromination (2) Review (3) Electron impact (4) PIMS detection	(1) 1973MEN/GOL (2) 1983WEI/BEN (3) 1988HOL/LOS (4) 1991HUD/JON
dichloromethane $CHCl_2$–**H** $\Delta_f H^o(R)$ = 22.3±1.0 (93.3±4.2)	(1) 99.0±2 (2) 98.4±1.2 (3) 97.2±2 (4) 96.2±0.6 (5) **97.3±1.0**	414.2±8.4 411.7±5.0 406.7±8.4 402.5±2.7 **407.1±4.2**	(1) Toluene carrier tech. (2) Bromination (3) Electron impact (4) PIMS detection (5) Review	(1) 1958PRI/TRO (2) 1987TSC/PAD (3) 1988HOL/LOS (4) 1996SEE (5) 1997POU/PAU
chloromethane CH_2Cl–**H** $\Delta_f H^o(R)$ = 28.0±0.7 (117.2±2.9)	(1) 100.8±1 (2) 99.4±2 (3) **100.1±0.6** (4) 100±2 (5) 99.9	421.7±4.2 415.9±8.4 **419.0±2.3** 418.4±8.4 418	(1) Bromination (2) Electron impact (3) PIMS detection (4) Review (5) FT-ICR	(1) 1987TSC/PAD (2) 1988HOL/LOS (3) 1996SEE (4) 1997POU/PAU (5) 2000BOR/ING
bromochloromethane CHBrCl–**H** $\Delta_f H^o(R)$ = 36.8±3 (154.0±13)	**93.9** 91.3	**393** 382.0	FT-ICR	2000BOR/ING
tribromomethane CBr_3–**H** $\Delta_f H^o(R)$ = 49.0±2 (205.0±8.4)	(1) 96.0±1.6 (2) 95.4±2	401.7±6.7 399.2±8.4	(1) Bromination (2) Electron impact	(1) 1971KIN/GOL (2) 1988HOL/LOS
dibromomethane $CHBr_2$–**H** $\Delta_f H^o(R)$ = 45.0±2.2 (188.3±9.2)	(1) 103.7±2 (2) **99.7±1.8** (3) 97.9±2 (4) 98.2	433.9±8.4 **417.1±7.5** 409.6±8.4 411	(1) Toluene carrier tech. (2) Bromination (3) Electron impact (4) Review	(1) 1958PRI/TRO (2) 1987TSC/PAD (3) 1988HOL/LOS (4) 2000BOR/ING

(continued)

Table 3.5 (continued) C–H BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
bromomethane CH_2Br–**H** $\Delta_f H^o(R) = 40.4 \pm 1$ (169.0±4.2)	(1) 102.0±2 (2) **101.6±1** (3) 100.8±2	426.8±8.4 **425.1±4.2** 421.7±8.4	(1) Toluene carrier tech. (2) Bromination (3) Electron impact	(1) 1958PRI/TRO (2) 1987TSC/PAD (3) 1988HOL/LOS
diiodomethane CHI_2–**H** $\Delta_f H^o(R) = 79.8 \pm 2.2$ (333.9±9.2)	103±2	431.0±8.4	Review	1970ONE/BEN
iodomethane CH_2I–**H** $\Delta_f H^o(R) = 54.9 \pm 2$ (229.7±8.4)	(1) 103±2 (2) 103.5±2 (3) 103.2±0.7	431.0±8.4 433.0±8.4 431.6±2.8	(1) Review (2) Electron impact (3) Kinetics	(1) 1970ONE/BEN (2) 1988HOL/LOS (3) 2002SEE
pentafluoroethane CF_3CF_2–**H** $\Delta_f H^o(R) = -213.4 \pm 1$ (–892.9±4.2)	(1) 103.1±1.5 (2) **102.7±0.5**	431.4±6.3 **429.7±2.1**	(1) Kinetics (2) Photolysis	(1) 1972BAS/WHI (2) 1981EVA/WHI
1,1,2,2-tetrafluoroethane CHF_2CF_2–**H** $\Delta_f H^o(R) = -158.9 \pm 4.5$ (–664.8±18.8)	103.0±4.5	431.0±18.8	Review	1996ZAR/WES
1,2,2-trifluoroethane CH_2FCF_2–**H** $\Delta_f H^o(R) = -107.5 \pm 3.5$ (–449.8±14.6)	103.5±3.5	433.0±14.6	Review	1996ZAR/WES

1,2,2-trifluoroethane CHF_2CFH–**H** $\Delta_fH^o(R) = -109\pm3.5$ (-456.1 ± 14.6)	102.0±3.5	426.8±14.6	Review	1996ZAR/WES
1,1,1-trifluoroethane CF_3CH_2–**H** $\Delta_fH^o(R) = -123.6\pm2$ (-517.1 ± 8.4)	106.7±1.1	446.4±4.5	Kinetics	1974WU/ROD
1,1-difluoroethane CH_3CF_2–**H** $\Delta_fH^o(R) = -72.3\pm2$ (-302.5 ± 8.4)	99.5±1	416.3±4.2	Iodination	1977PIC/ROD
1,2-difluoroethane CH_2FCHF–**H** $\Delta_fH^o(R) = -57.0\pm3$ (-238.5 ± 12.6)	98.8±3	413.4±12.6	UV-flash photolysis	1983MAR/PAR
1,1-difluoroethane CHF_2CH_2–**H** $\Delta_fH^o(R) = -68.3\pm3.5$ (-285.8 ± 14.6)	103.5±3.5	433.0±14.6	Review	1996ZAR/WES
fluoroethane CH_2FCH_2–**H** $\Delta_fH^o(R) = -14.2\pm2$ (-59.4 ± 8.4)	(1) **103.6±2** (2) 100.8±2	**433.5±8.4** 421.7±8.4	(1) Review (2) Photobromin.	(1) 1996ZAR/WES (2) 1996MIY/OZA
fluoroethane CH_3CHF–**H** $\Delta_fH^o(R) = -16.8\pm2$ (-70.3 ± 8.4)	(1) 97.3±2 (2) **98.2±2**	407.1±8.4 **410.9±8.4**	(1) Bromination (2) Photobromin.	(1) 1987TSC/SAL(b) (2) 1996MIY/OZA
1-chloro-2,2,2-trifluoro-ethane CF_3CHCl–**H**	101.8±1.5	425.9±6.3	Review	1982MCM/GOL

(continued)

Table 3.5 (continued) C–H BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-bromo-1-chloro-2,2, 2-trifluoroethane CF_3CClBr–**H** $\Delta_f H^o(R) = -120.5 \pm 2$ (–504.2±8.4)	96.6±1.5	404.2±6.3	Review	1982MCM/GOL
2-chloro-1,2,2-trifluoro-ethane $CClF_2CHF$–**H** $\Delta_f H^o(R) = -107.7 \pm 3$ (–450.6±12.6)	98.5±0.5	412.1±2.1	Pyrolysis	1998SKO/DYM
pentachloroethane CCl_3CCl_2–**H** $\Delta_f H^o(R) = 8.4 \pm 1.3$ (35.1±5.4)	(1) 95.8 (2) 95±2	400.8 397.5±8.4	(1) Photochlorin. (2) Shock tube	(1) 1969FRA/HUY (2) 1976LEW
1,1,2,2-tetrachloroethane $CHCl_2CCl_2$–**H** $\Delta_f H^o(R) = 5.6 \pm 2$ (23.4±8.4)	94±2	393.3±8.4	Shock tube	1976LEW
1,1-dichloroethane CH_3CCl_2–**H** $\Delta_f H^o(R) = 10.2 \pm 0.4$ (42.7±1.7)	(1) 93.4±0.4 (2) 95.1±1.2	390.6±1.5 397.9±5.0	(1) PIMS detection (2) Kinetics	(1) 1996SEE (2) 1999MIY/TSC
chloroethane CH_3CHCl–**H** $\Delta_f H^o(R) = 18.3 \pm 0.4$ (76.6±1.5)	(1) 95.7 (2) 98.2±2 (3) 96.5±1 (4) **97.2±0.4**	400.4 410.9±8.4 403.8±4.2 **406.6±1.5**	(1) Bromination (2) Electron impact (3) Photobromin. (4) PIMD detection	(1) 1987TSC/SAL(b) (2) 1988HOL/LOS (3) 1990MIY/TSC (4) 1996SEE

chloroethane CH_2ClCH_2–**H** $\Delta_fH^o(R)$ = 22.2±0.6 (93.0±2.4)	(1) 101.7±2 (2) 100.7±1 (3) **101.1±0.6**	425.5±8.4 421.3±4.2 **423.1±2.4**	(1) Electron impact (2) Photobromin. (3) PIMS detection	(1) 1988HOL/LOS (2) 1990MIY/TSC (3) 1998SEE
1,1-dibromoethane CH_3CBr_2–**H** $\Delta_fH^o(R)$ = 33.5±1.3 (140.2±5.4)	94.9±1.2	397.1±5.0	Kinetics	1999MIY/TSC
bromoethane CH_2BrCH_2–**H** $\Delta_fH^o(R)$ = 32.3 (135.1)	99.2±2	415.1±8.4	Electron impact	1988HOL/LOS
bromoethane CH_3CHBr–**H** $\Delta_fH^o(R)$ = 30.3 (126.8)	(1) 96.4 (2) 94.2±2 (3) **97.2±1**	403.3 394.1±8.6 **406.7±4.2**	(1) Bromination (2) Electron impact (3) Photobromin.	(1) 1987TSC/SAL(b) (2) 1988HOL/LOS (3) 1990MIY/TSC
trifluoroethylene CF_2=CF–**H**	111.0±2.0	464.4±8.4	Correlation	1981STE/ROW
1,1-difluoroethylene CF_2=CH–**H** $\Delta_fH^o(R)$ = –22.2±2 (–92.9±8.4)	110±2	460.2±8.4	Correlation	1981STE/ROW
(Z)-1,2-difluoroethylene CHF=CF–**H** $\Delta_fH^o(R)$ = –12.1±2 (–50.6±8.4)	110±2	460.2±8.4	Correlation	1981STE/ROW
1,1-difluoro-2-chloroethylene CF_2=CCl–**H**	109±2	456.1±8.4	Correlation	1981STE/ROW

(continued)

Table 3.5 (continued) C–H BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
(E)-1,2-chloro-2-fluoro-ethylene $CFCl{=}Cl{-}\mathbf{H}$	108±2	451.9±8.4	Correlation	1981STE/ROW
(Z)-1,2-dichloroethylene $CHCl = CCl{-}\mathbf{H}$ $\Delta_f H^o(R) = 56.1\pm2$ (234.7±8.4)	107±2	447.7±8.4	Correlation	1981STE/ROW
chloroethylene $CH_2 = CCl{-}\mathbf{H}$ $\Delta_f H^o(R) > 60.4$ (>252.7)	>103.6	>433.5	PIMS detection	1989RUS/SEN
1,1,1,2,2,3,3-heptafluoro-propane $CF_3CF_2CF_2{-}\mathbf{H}$	(1) 104±2 (2) 103.3	435.1±8.4 432.2	(1) Review (2) Bromination	(1) 1982MCM/GOL (2) 1983EVA/WEE
1,1,1,2,3,3,3-heptafluoro-propane $CF_3CF\mathbf{H}CF_3$	103.5±0.6	433.0±2.5	Kinetics	1983EVA/WEE
1-chloropropane $CH_3CH_2CHCl{-}\mathbf{H}$ $\Delta_f H^o(R) = 13.5\pm0.8$ (56.6±3.3)	97.3±0.8	407.0±3.5	Derived	1998SEE
1-chloropropane $CH_2ClC\mathbf{H}_2CH_3$	97.8±0.9	409.3±3.9	Derived	1998SEE
1-fluoropropene $CH_2 = CH\text{-}CHF{-}\mathbf{H}$	88.6±1.1	370.7±4.6	VLPP	1973ALF/GOL

1-chloropropene CH_2 = CH-CHCl–**H**	88.6±1.1	370.7±4.6	VLPP	1973ALF/GOL
1-bromopropene CH_2 = CH-CHBr–**H** $\Delta_f H^o(R)$ = 48.1±1.1 (201.3±4.6)	89.4±1.1	374.0±4.6	VLPP	1973ALF/GOL
pentafluorobenzene C_6F_5–**H** $\Delta_f H^o(R)$ = –130.9±2 (–547.7±8.4)	113.9	476.6	Toluene carrier tech.	1974KRE/PRI
9-pentafluorophenyl fluorine 9-C_6F_5Fl**H**	78.2	327.2	AOP	1993BOR/ZHA(b)
tri(2,3,5,6-tetrafluoro-phenyl)phenyl methane (p–$HC_6F_4)_3$C**H**	82.3	344.3	AOP	1993BOR/ZHA(b)

3.6 Organic compounds containing heteroatoms

3.6.1 C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

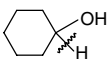
Table 3.6.1 C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	 kJ/mol	Methods (references in parentheses)	References
methanol **H**–CH_2OH $\Delta_f H^o(R)$ = –4.08±0.8 (–17.07±3.35)	(1) 95.9±1.5 (2) 96.0 (3) 96.2±0.2 (4) **96.06±0.15** (5) 96.2±0.3	401.2±6.3 401.7 402.5±0.8 **401.92±0.63** 402.5±1.3	(1) Iodination (2) SPST (3) PIMS detect. (4) Recommend. (5) Resonance fluorescence	(1) 1973ONE/BEN (2) 1981TSA (3) 1993RUS/BER (4) 1994BER/ELL (5) 1996DOB/BER
ethanol CH_3CH_2OH	(1) 93±1.0 (2) 94.6	389.1±4.2 395.8	(1) Iodination (2) SPST	(1) 1973ALF/GOL (2) 1981TSA

(continued)

Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$\Delta_f H^o(R) = -13.3 \pm 0.8$ (–55.6±3.5)	(3) **94.8**	**396.6**	(3) Electron impact	(3) 1991HOL/LOS
	(4) 98±2	410.0±8.4	(4) PIMS detect.	(4) 1994RUS/BER
	(5) 95.9±1	401.2±4.2	(5) Review	(5) 1999ATK/BAU
ethanol $C\mathbf{H}_3CH_2OH$ $\Delta_f H^o(R) = -7.0$ (–29.3)	101.3	423.8	MS	1990TAK
propanol $CH_3CH_2C\mathbf{H}_2OH$ $\Delta_f H^o(R) = -19.4 \pm 1$ (–81±8)	(1) 93.7	392.0	(1) SPST	(1) 1999TSA
	(2) 93.2	389.9	(2) Correlation	(2) 2000DEN/DEN
propanol $CH_3CH_2C\mathbf{H}_2OH$ $\Delta_f H^o(R) = -18.8 \pm 2$ (–78.7±8.4)	94.3±2	394.6±8.4	AE	1992HOL
propanol $C\mathbf{H}_3CH_2CH_2OH$ $\Delta_f H^o(R) = -16.0 \pm 2$ (–66.9±8.4)	97.1±2	406.3±8.4	AE	1992HOL
propan-2-ol $(CH_3)_2C\mathbf{H}OH$ $\Delta_f H^o(R) = -26.3 \pm 1$ (–110.0±4.2)	(1) **91±1**	**380.7±4.2**	(1) Review	(1) 1982MCM/GOL
	(2) 89.3±1.7	373.6±7.1	(2) PAC	(2) 1989KAM/GRI
	(3) 91.7±2	383.7±8.4	(3) AE	(3) 1992HOL
	(4) 93.0	389.1	(4) Correlation	(4) 2000DEN/DEN
propan-2-ol $(C\mathbf{H}_3)_2CHOH$ $\Delta_f H^o(R) = -23.0 \pm 1$ (–96.2±4.2)	94.3±2	394.6±8.4	AE	1992HOL

allyl alcohol CH_2=CHC**H**$_2$OH $\Delta_f H^o(R) = 0 \pm 2$ (0±8.4)	(1) **81.6±1.8** (2) 80.1 (3) 85.2	**341.4±7.5** 355.1 356.5	(1) Iodination (2) PAC (3) Correlation	(1) 1973ALF/GOL (2) 1992ARN/CAL (3) 2000DEN/DEN
2-methylpropan-2-ol (C**H**$_3$)$_3$COH $\Delta_f H^o(R) = -26.8 \pm 2$ (–112.1±8.4)	(1) 100.0±2.0 (2) 99.1 (3) 100.0	418.4±8.4 414.6 418.6	(1) Review (2) APC (3) Correlation	(1) 1982MCM/GOL (2) 1989KAM/GRI (3) 2000DEN/DEN
penta-1,4-dien-3-ol (CH_2=CH)$_2$C**H**OH $\Delta_f H^o(R) = 22.1 \pm 2$ (92.5±8.4)	89	372.4	PAC	1991CLA/CUL
cyclohexanol  	92.4	386.7	Correlation	2000DEN/DEN
benzyl alcohol C_6H_5C**H**$_2$OH	87.5	366.3	Correlation	2000DEN/DEN
1-phenylethanol PhMeC(OH)–**H**	88.3	369.4	Correlation	2000DEN/DEN
diphenylmethn-1-ol Ph_2C**H**OH $\Delta_f H^o(R) = 36.4 \pm 1.5$ (152.3±6.3)	75.4±1.5	315.5±6.3	PAC	1992ARN/CAL
ethane-1,2-diol (C**H**$_2$OH)$_2$ $\Delta_f H^o(R) = -52.6 \pm 2$ (–220.1±8.4)	(1) 89.6±2.2 (2) **92.1** (3) 95.6	374.9±9.2 **385.3** 400.0	(1) PAC (2) AE (3) Correlation	(1) 1989KAM/GRI (2) 1992HOL (3) 2000DEN/DEN

(continued)

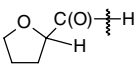
Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1,4-butanediol $HOCH_2(CH_2)_2(OH)CH–\mathbf{H}$	95.4	399.2	Correlation	2000DEN/DEN
dimethyl ether $C\mathbf{H}_3OCH_3$ $\Delta_f H^o(R) = 0\pm1$ (0±4.2)	(1) 95.5 (2) 93±1 (3) **96.1** (4) 95.3	399.6 389.1 **402.1** 398.7	(1) Photodissocn. (2) Review (3) Review (4) Correlation	(1) 1967LOU/LAI (2) 1969GOL/BEN (3) 1999ATK/BAU (4) 2000DEN/DEN
difluoromethyl trifluoromethyl ether $C\mathbf{H}F_2OCF_3$	106±1	443.5±4.2	Kinetics	1995HSU/DEM
bis(difluoromethyl) ether $C\mathbf{H}F_2OCHF_2$	104±1	435.1±4.2	Kinetics	1995HSU/DEM
methyl trifluoromethyl ether $C\mathbf{H}_3OCF_3$	102±1	426.8±4.2	Kinetics	1995HSU/DEM
ethyl methyl ether $C\mathbf{H}_3OCH_2CH_3$ $\Delta_f H^o(R) = -10.8\pm2$ (–45.2±8.4)	93.0	389.1	AE	1991HOL/LOS
diethyl ether $CH_3C\mathbf{H}_2OCH_2CH_3$ $\Delta_f H^o(R) = -19.4\pm1$ (–81.2±4.2)	(1) 91.7±0.4 (2) **93** (3) 94.8	383.7±1.7 **389.1** 396.5	(1) VLPP (2) PAC (3) Correlation	(1) 1984KON/BEN (2) 1986BUR/MAJ (3) 2000DEN/DEN
diisopropyl ether $(CH_3)_2C\mathbf{H}OCH(CH_3)_2$	(1) 93.9 (2) 90.4	392.9 378.2	(1) Reanal. of pyrolysis data (2) Correlation	(1) 1998BRO/BEC (2) 2000DEN/DEN

ethyl tert-butyl ether $CH_3C\mathbf{H}_2Ot–C(CH_3)_3$	96.9	405.4	Reanal. of pyrolysis data	1998BRO/BEC
dibenzyl ether $PhC\mathbf{H}_2OCH_2Ph$	84.8	354.6	Correlation	2000DEN/DEN
cyclohexyl methyl ether cyclo-$C_6\mathbf{H}_{11}$–OMe	89.9	376.3	Correlation	2000DEN/DEN
dimethoxymethane $(MeO)_2C\mathbf{H}_2$	92.9	388.7	Correlation	2000DEN/DEN
1,1-dimethoxyethane $(MeO)_2Cme\mathbf{H}$	88.2	368.9	Correlation	2000DEN/DEN
Oxirane  $\Delta_fH^o(R) = 35.8\pm1.5$ (149.8 ± 6.3)	100.5±1.5	420.5±6.5	Pyrolysis	1984BAL/KEE
tetrahydrofuran  $\Delta_fH^o(R) = -4.3\pm1.5$ (-18.0 ± 6.3)	(1) 92±1 (2) **92.1±1.6** (3) 92	384.9±4.2 385.3±6.7 **384.9**	(1) Kinetics (2) PAC (3) PAC	(1) 1982MCM/GOL (2) 1997LAA/MUL (3) 2000KRA/CIR
formaldehyde HCO–**H** $\Delta_fH^o(R) = 9.96\pm0.20$ (41.67 ± 0.84)	(1) 87.0±1.0 (2) 88.8±0.5 (3) 88.0 (4) **88.04±0.16** (5) 88.6±0.1	364.0±4.2 371.5±2.1 368.2 **368.40±0.67** 370.86±0.28	(1) Iodination (2) Electron impact (3) Photolysis (4) Recommend. (5) Laser flash photolysis	(1) 1982MCM/GOL (2) 1985TRA (3) 1987CHU/FOL (4) 1994BER/ELL (5) 1997BEC/CAR

(continued)

Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

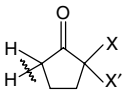
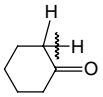
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
formyl fluoride FCO–**H**	101.1	423.0	Derived from $\Delta_f H^o$ in ref.	1998CHA
ethanal or acetadehyde CH_3CO–**H** $\Delta_f H^o(R) = -2.4 \pm 0.2$ (-10.0 ± 0.8)	(1) 87.1±1.3 (2) 87.3±2.0 (3) 89.3±0.5 (4) **89.4±0.3** (5) 88.7	364.4±5.4 365.3±8.4 373.6±2.1 **374.0±1.3** 371.1	(1) Iodination (2) Electron impact (3) PIMS detect. (4) Recommend. (5) SPST	(1) 1973ONE/BEN (2) 1984HOL/LOS (3) 1992NII/GUT (4) 1994BER/ELL (5) 1999TSA
trifluoroacetadehyde CF_3CO–**H**	91±2	380.7±8.4	Bromination	1970AMP/WHI
propanal C_2H_5CO–**H** $\Delta_f H^o(R) = -7.7 \pm 1$ (-32.3 ± 4.2)	(1) 87.4±1.0 (2) 89.5 (3) **88.7**	365.7±4.2 374.5 **371.1**	(1) Kinetics (2) Electrochem. (3) Derived	(1) 1973WAT/THO (2) 1995LUN/DAA (3) 2000ATK/BAU
propenal CH_2=CHCO–**H** $\Delta_f H^o(R) = 15.3 \pm 2$ (64.0 ± 8.4)	(1) 87±1 (2) **89.1**	364.0±4.2 **372.8**	(1) Iodination (2) Electrochem.	(1) 1973ALF/GOL (2) 1995LUN/DAA
furfurol 	90.5	378.7	Correlation	2000DEN/DEN
benzaldehyde C_6H_5CO–**H** $\Delta_f H^o(R) = 27.8 \pm 2.6$ (116.3 ± 10.9)	(1) 86.9±1.0 (2) **88.7±2.6** (3) 88.9	363.6±4.2 **371.1±10.9** 372.0	(1) Iodination (2) PAC (3) Electrochem.	(1) 1982MCM/GOL (2) 1989SIM/GRI (3) 1995LUN/DAA

ketene **H**–CH=C=O $\Delta_f H^o(R) = 41.9 \pm 2$ (175.3±8.4)	105.3±2.1	440.6±8.8	Recommend.	1994BER/ELL
acetone C**H**$_3$COCH$_3$ $\Delta_f H^o(R) = -8.1 \pm 0.7$ (–33.9±3)	(1) 98.3±1.8 (2) 92±2 (3) 94 (4) 100.9 (5) **95.9±0.7**	411.3±7.5 384.9±8.4 393.3 422.2 **401.2±2.9**	(1) Bromination (2) AE (3) AOP (4) SPST (5) Derived from $\Delta_f H^o(R)$ in ref.	(1) 1970KIN/GOL (2) 1984HOL/LOS(b) (3) 1990BOR/HAR (4) 1999TSA (5) 2001BOU/CHA
ethyl methyl ketone MeCOC**H**$_2$Me $\Delta_f H^o(R) = -16.8 \pm 1.7$ (–70.3±7.1)	(1) 92.3±1.7 (2) 94.0	386.2±7.1 393.3	(1) Iodination (2) Correlation	(1) 1970SOL/GOL (2) 2000DEN/DEN
diethyl ketone EtCOC**H**$_2$Me $\Delta_f H^o(R) = -25.7 \pm 5$ (–107.5±20.9)	88	368.2	AOP	1990BOR/HAR
methyl tert-butyl ketone C**H**$_3$COtBu $\Delta_f H^o(R) = -27.6 \pm 3$ (–115.5±12.6)	94	393.3	AOP	1990BOR/HAR
diiso-propyl ketone Me$_2$CHCOC**H**Me$_2$ $\Delta_f H^o(R) = -41.5 \pm 5$ (–173.6±20.9)	(1) 85 (2) 93.6	355.6 391.5	(1) AOP (2) Correlation	(1) 1990BOR/HAR (2) 2000DEN/DEN
methyl phenyl ketone C**H**$_3$COPh $\Delta_f H^o(R) = 20.2 \pm 3$ (84.5±12.6)	(1) 93 (2) 90.7	389.1 379.6	(1) AOP (2) Correlation	(1) 1990BOR/ZHA (2) 2000DEN/DEN
methyl p-NO$_2$-phenyl ketone C**H**$_3$CO(p-NO$_2$–C$_6$H$_4$)	89	372.0	AOP	1995ZHA/BOR

(continued)

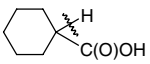
Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
ethyl phenyl ketone Me**CH**$_2$COPh $\Delta_f H^o(R)$ = 9.9±5 (41.4±20.9)	(1) 88 (2) 89.4 (3) 92.9	368.2 374.2 388.7	(1) AOP (2) Correlation (3) Reanal. of pyrolysis data	(1) 1990BOR/HAR (2) 2000DEN/DEN (3) 1998BRO/BEC
benzyl methyl ketone Ph**CH**$_2$COMe	82.3	344.3	AOP	1992BOR/JI
benzyl phenyl ketone Ph**CH**$_2$COPh	82.5	345.2	AOP	1990BOR/HAR
dibenzyl ketone Ph**CH**$_2$COCH$_2$Ph $\Delta_f H^o(R)$ = 32.1±3 (134.3±12.6)	(1) 83 (2) 87.1	347.3 364.5	(1) AOP (2) Correlation	(1) 1990BOR/HAR (2) 2000DEN/DEN
propylphenyl phenyl ketone Ph**CH**$_2$CH$_2$COPh	88.5	370.3	AOP	1990BOR/HAR
iso-propyl phenyl ketone PhCOC**H**Me$_2$	(1) 86 (2) 87.2 (3) 89.9	359.8 365.0 376.1	(1) AOP (2) Correlation (3) Reanal. of pyrolysis data	(1) 1990BOR/HAR (2) 2000DEN/DEN (3) 1998BRO/BEC
diphenylmethyl methyl ketone Ph$_2$C**H**COCH$_3$	82	343.1	AOP	1990BOR/HAR
diphenylmethyl phenyl ketone Ph$_2$C**H**COPh	83	347.3	AOP	1990BOR/HAR

cyclopentanone, substituted  $\Delta_f H^o$ (cyclopentanonyl) = –10±3 (–41.8±12.6) X = H, X′ = H	(1) 88 (2) 94.8	368.2 396.5	(1) AOP (2) Correlation	(1) 1991BOR/GAL (2) 2000DEN/DEN
Me Me	(1) 89	372.4		
cyclohexanone 	94.1	393.9	Correlation	2000DEN/DEN
formic acid **H**–C(O)OH $\Delta_f H^o$(R) = –46.5±0.7 (–194.6±2.9)	(1) 98 (2) 93.2 (3) >89.5 (4) **96.6** (5) 97.4±0.7	410.0 389.9 >374.5 **404.2** 407.5±2.9	(1) Correlation (2) Electron impact (3) Review (4) Review (5) Gas-phase basicity	(1) 1973MCK/DUN (2) 1991HOL/LOS (3) 1994BER/ELL (4) 1994BER/ELL (5) 2000RUS/LIT
acetic ion C**H**$_3$C(O)O$^-$	(1) 91.9±1.7 (2) 96.1 (3) ~95	384.5±7.1 402.0 ~397.5	(1) APC (2) Derived (3) Review	(1) 1989KAM/GRI (2) 1994YU/RAU (3) 2002REE/KAS
acetic acid C**H**$_3$C(O)OH $\Delta_f H^o$(R) = –60.2±2.9 (–251.9±12.0)	(1) 96.1 (2) 93.9±2.0 (3) **95.3±2.9** (4) 95.9 (5) 98.7±0.8	402.1 392.9±8.4 **398.7±12.1** 401.3 413.0±3.3	(1) Correlation (2) AE (3) CID (4) Correlation (5) Calorimetry	(1) 1984NON/WAL (2) 1991HOL/LOS (3) 1994WEN/SQU (4) 2000DEN/DEN (5) 2001LAG/DIO
chloroacetic acid ClC**H**$_2$C(O)OH	(1) 95.3 (2) 91.0±0.9	398.7 380.7±3.9	(1) Correlation (2) Combination	(1) 2000DEN/DEN (2) 2002LAG/DIO
propanoic acid CH$_3$C**H**$_2$C(O)OH	95.3	398.8	Correlation	2000DEN/DEN

(continued)

Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-methyl propanoic acid $(CH_3)_2C\mathbf{H}C(O)OH$	93.0	389.0	Correlation	2000DEN/DEN
cyclohexacarboxylic acid 	93.0	389.0	Correlation	2000DEN/DEN
benzenacetic acid $PhC\mathbf{H}_2C(O)OH$	87.9	367.8	Correlation	2000DEN/DEN
glycolic acid $(OH)C\mathbf{H}_2C(O)OH$	92.6	387.5	Correlation	2000DEN/DEN
2,2-dimethyl-propanoic acid $(C\mathbf{H}_3)_3CC(O)OH$	99.2	415.1	Correlation	2000DEN/DEN
methyl formate $\mathbf{H}$–$C(O)OCH_3$ $\Delta_f H^o(R) = -40.5 \pm 2$ (-169.5 ± 8.4)	(1) 92.7±1 (2) 95.4	387.9±4.2 399.2	(1) Kinetics (2) Electron impact	(1) 1969SOL/BEN (2) 1991HOL/LOS
acetic acid methyl ester $C\mathbf{H}_3C(O)OCH_3$ $\Delta_f H^o(R) = -56.6 \pm 2$ (-236.8 ± 8.4)	(1) 93.9 (2) 97.1±2.5	392.9 406.3±10.5	(1) Electron impact (2) FT-ICR	(1) 1991HOL/LOS (2) 2002KAR/JAN
acetic acid methyl ester $CH_3C(O)OC\mathbf{H}_3$	96.7	404.6	Correlation	2000DEN/DEN

acetic acid ethyl ester C**H**$_3$C(O)OCH$_2$CH$_3$ $\Delta_f H^o(R) = -62.2 \pm 3$ (-260.2 ± 12.6)	(1) 96 (2) 95.4	401.7 399.5	(1) AOP (2) Correlation	(1) 1995BOR/ZHA (2) 2000DEN/DEN
acetic acid isopropyl ester CH$_3$C(O)OC**H**(CH$_3$)$_2$	93.8	392.3	Correlation	2000DEN/DEN
acetic acid phenyl ester C**H**$_3$C(O)OPh $\Delta_f H^o(R) = -16.7(-69.9)$	100.2±1.3	419.2±5.4	Iodination	1973ALF/GOL
oxalic acid dimethyl ester CH$_3$C(O)OC(O)OC**H**$_3$	96.5	403.8	Correlation	2000DEN/DEN
acetic acid anhydride CH$_3$C(O)OC(O)C**H**$_3$	97.0	406.0	Correlation	2000DEN/DEN
ethyl propanoate CH$_3$C**H**$_2$C(O)OEt	95.6	400.0	Reanal. of pyrolysis data	1998BRO/BEC
ethyl 2-phenylacetate PhC**H**$_2$C(O)OEt	(1) 84.0 (2) 88.6	351.5 370.7	(1) AOP (2) Reanal. of pyrolysis data	(1) 1994ZHA/BOR(e) (2) 1998BRO/BEC
2-methoxy-1-phenylethan-1-one PhCOC**H**$_2$OMe	81	338.9	AOP	1990BOR/HAR
2-ethoxy-1-phenylethan-1-one PhCOC**H**$_2$OEt	80.6	337.2	AOP	1994BOR/ZHA

(continued)

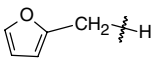
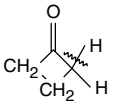
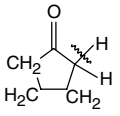
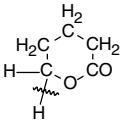
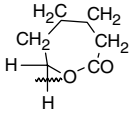
Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

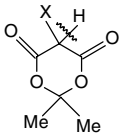
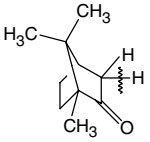
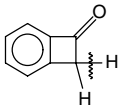
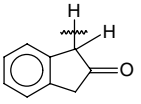
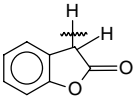
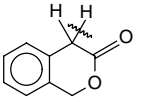
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-phenyl-2-phenoxyethan-1-one PhCOC**H**$_2$OPh	80.6	337.2	AOP	1994BOR/ZHA
pentane-2,4-dione C**H**$_2$(COMe)$_2$	(1) 91.6 (2) 87.7	383.3 366.9	(1) AOP (2) Reanal. of pyrolysis data	(1) 1995BOR/ZHA (2) 1998BRO/BEC
1,3-diphenylpropane-1,3-dione C**H**$_2$(COPh)$_2$	(1) 93 (2) 92	389.1 384.9	AOP	(1) 1990BOR/HAR (2) 1991BOR/HAR
ethyl methyl butane-1,4-dioate C**H**$_2$(COMe)(C(O)OEt)	92.9	388.7	AOP	1995BOR/ZHA
malonic acid dimethyl ester C**H**$_2$(MeOC(O))$_2$	(1) 90.5 (2) 93.3	378.7 390.4	(1) AOP (2) Correlation	(1) 1991BAU/FAS(c) (2) 2000DEN/DEN
ethyl methyl propane-1,3-dioate C**H**$_2$(C(O)OEt)(C(O)OMe)	92.3	386.2	AOP	1996ZHA/BOR
oxilic axcid diethyl ester C**H**$_2$(C(O)OEt)$_2$	(1) 95.0 (2) 94.8	397.5 396.5	(1) AOP (2) Correlation	(1) 1993ZHA/BOR (2) 2000DEN/DEN
1-phenylbutane-1,3-dione PhCOC**H**$_2$COMe	92	384.9	AOP	1990BOR/HAR

3-methylpentane-2,4-dione (Me)C**H**$(COMe)_2$	84.7	354.4	Reanal. of pyrolysis data	1998BRO/BEC
dimethyl 2-methyl propane-1,3-dioate MeC**H**$(C(O)OMe)_2$	(1) 90.5 (2) 90.8	378.7 379.9	AOP	(1) 1994ZHA/BOR(e) (2) 1996ZHA/BOR
ethyl 2-methylpropanoate Me_2C**H**C(O)OEt	92.6	387.4	Reanal. of pyrolysis data	1998BRO/BEC
ethyl methyl 2-ethyl propane-1,3-dioate EtC**H**(C(O)OEt)(C(O)OMe)	89.6	374.9	AOP	1996ZHA/BOR
diethyl 2-ethyl propane-1, 3-dioate EtC**H**$(C(O)OEt)_2$	91.5	382.8	AOP	1996ZHA/BOR
oxilic acid bis(1-methylethyl) ester $(Me_2$C**H**C(O)O$)_2$	93.9	392.9	Correlation	2000DEN/DEN
diethoxy 2-phenylpropane-1, 3-dione PhC**H**$(C(O)OEt)_2$	85.3	356.9	AOP	1993ZHA/BOR
ethyl 2-phenylpropanoate PhC**H**Me(C(O)OEt)	85.6	358.2	Reanal. of pyrolysis data	1998BRO/BEC
diethyl 2-(1,1-dimethyl-1silaethyl) propane-1,3-dioate Me_3SiCH_2C**H**$(CO_2Et)_2$	87.3	365.3	AOP	1996ZHA/BOR
ethyl methyl 2-(1,1-dimethyl-1silaethyl) propane-1,3-dioate Me_3SiC**H**$(CO_2Et)(CO_2Me)$	85.2	365.5	AOP	1996ZHA/BOR

(continued)

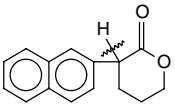
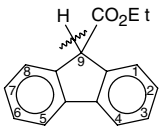
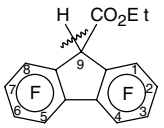
Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-methyl furan 	86.5±2	361.9±8.4	VLPP	1981STE
β-propiolactone 	99.4±2.3	415.9±9.6	FT-ICR	2002KAR/JAN
γ-butyrolactone 	94.8±2.3	396.6±9.6	FT-ICR	2002KAR/JAN
1,4-dioxane 				
$\Delta_f H^o(R)$ = –31.5±3 (–131.8±12.6)	(1) 96.0 (2) 96.6	401.7 404.3	(1) PAC (2) Correlation	(1) 2000KRA/CIR (2) 2000DEN/DEN
δ-valerolactone 	89.2±2.3	373.2±9.6	FT-ICR	2002KAR/JAN
ε-caprolactone 	92.8±2.4	388.3±10.0	FT-ICR	2002KAR/JAN

2,2-dimethyl-1,3-dioxae-4, 6-dione 				
X = H	92.6	387.4	AOP	1994ZHA/BOR(e)
Me	87.5	366.1		
1,7,7-trimethyl bicyclo(2.2.1) heptane-2-one 	95	397.5	AOP	1991BOR/JI
benzocyclobutenone 	90.5±3.1	378.7±13.0	FT-MS	1999BRO/KAS
indan-2-one 	79.1	331.0	AOP	1994ZHA/BOR(e)
3-hydrobenzo(b)furan-2-one 	80.1	335.1	AOP	1994ZHA/BOR(e)
isochroman-3-one 	83.4	348.9	AOP	1994ZHA/BOR(e)

(continued)

Table 3.6.1 (continued) C–H BDEs with α-OH, -OR, -C(O), and -C(O)O

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
3-(2-naphthyl)-3H-4,5, 6,-trihydropyran-2-one 	81.8	342.3	AOP	1994ZHA/BOR(e)
ethyl fluorene-9-carboxylate 	76.1	318.4	AOP	1993BOR/ZHA(b)
ethyl octafluoro-fluorene-9-carboxylate 	80.7	337.6	AOP	1993BOR/ZHA(b)

3.6.2 C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

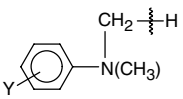
Table 3.6.2 C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
methylamine	(1) 93±2.5	389.1±10.5	(1) VLPP	(1) 1975KIN/GOL
$C\mathbf{H}_3NH_2$	(2) 96.6	404.2	(2) SPST	(2) 1981TSA
$\Delta_f H^o(R)$ = 36.3±2 (151.9±8.4)	(3) **93.9±2**	**392.9±8.4**	(3) Electron impact	(3) 1983BUR/CAS
	(4) 88.7	371.1	(4) VLPP	(4) 1984GRE/COL

2-azaprop-1-ene $CH_3N{=}CH_2$	97.5±3.5	407.9±14.6	VLPP	1993LAZ/PAP
ethylamine $CH_3CH_2NH_2$ $\Delta_fH^o(R)$ = 26.7±2 (111.7±8.4)	(1) 94.0 (2) **90.1±2** (3) 97.1	393.3 **377.0±8.4** 406.7	(1) SPST (2) Electron impact (3) Reanal. of pyrolysis data	(1) 1981TSA (2) 1983BUR/CAS (3) 1998BRO/BEC
triethylamine $(C_2H_5)_2NCH_2CH_3$ $\Delta_fH^o(R)$ = 16.4±0.5 (68.6±2.1)	(1) 85.0 (2) 91.0±2.4 (3) **90.7±0.4** (4) 89 (5) 91.2±2	355.6 381±10.0 **379.5±1.7** 372.4 381.6±8.4	(1) SPST (2) PAC (3) PAC (4) PAC (5) PAC	(1) 1981TSA (2) 1997WAY/CLA (3) 1999DOM/DIN (4) 2000KRA/CIR (5) 2002LAL/ALL
tributylamine $(nBu)_2NCH_2(nPr)$	(1) **91.0±2.4** (2) 89.5±2	**381±10.0** 374.5±8.4	PAC	(1) 1997WAY/CLA (2) 2002LAL/ALL
iso-propylamine $(CH_3)_2CHNH_2$ $\Delta_fH^o(R)$ = 16.7±2 (69.9±8.4)	(1) 95.2 (2) **88.9±2** (3) 94.2	398.3 **372.0±8.4** 394.1	(1) SPST (2) Electron impact (3) Reanal. of pyrolysis data	(1) 1981TSA (2) 1983BUR/CAS (3) 1998BRO/BEC
dimethylamine CH_3NHCH_3 $\Delta_fH^o(R)$ = 30.5±2 (127.6±8.4)	87±2	364.0±8.4	Electron impact	1981GRI/LOS
trimethylamine $(CH_3)_3N$ $\Delta_fH^o(R)$ = 33.2±2 (138.9±8.4)	(1) 84±2 (2) 87.0±1.0 (3) 87.5 (4) 88.9±2.4 (5) **91**	351.5±8.4 364.0±4.2 366.1 372±10.0 **380.7**	(1) Electron impact (2) VLPP (3) PAC (4) PAC (5) PAC, revised	(1) 1981GRI/LOS (2) 1984GRE/COL (3) 1993CLA/WAY (4) 1997WAY/CLA (5) 1999LAA/MUL
tert-butyldimethylamine $t\text{-}BuN(CH_3)_2$	90.0±1.2	376.6±5.0	PAC	1999DOM/DIN

(continued)

Table 3.6.2 (continued) C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

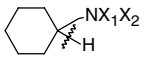
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
phynelmethylamine $PhC\mathbf{H}_2NH_2$	88.0	368.2	Correlation	2000DEN/KHU
dimethylbenzylamine $PhC\mathbf{H}_2N(CH_3)_2$	84.9	355.3	Correlation	2000DEN/KHU
phenyldiethylamine $PhN(C\mathbf{H}_2CH_3)_2$	91.6±1.0	383.3±4.2	PAC	1999DOM/DIN
diphenylmethylamine $Ph_2NC\mathbf{H}_3$	90.7±0.4	379.5±1.7	PAC	1999DOM/DIN
phenyldibenzylamine $PhN(C\mathbf{H}_2Ph)_2$	85.4±2.1	357.3±8.8	PAC	1999DOM/DIN
tribenzylamine $N(C\mathbf{H}_2Ph)_3$	(1) 89.1±0.6 (2) 86.3	372.8±2.5 361.1	(1) PAC (2) Correlation	(1) 1999DOM/DIN (2) 2000DEN/KHU
phenyldiallylamine $PhN(C\mathbf{H}_2CH{=}CH_2)_2$	81.1±0.7	339.3±2.9	PAC	1999DOM/DIN
triallylamine $N(C\mathbf{H}_2CH{=}CH_2)_3$	82.6±0.8	345.6±3.3	PAC	1999DOM/DIN
N,N-dimethylaniline, substituted 				

Y = H $\Delta_f H^o$(R, for Y = H) = 63.6±3 (266.1±12.6)	(1) 91.7±1.3 (2) 85.7	383.7±5.4 358.4	(1) PAC (2) Correlation	(1) 1999DOM/DIN (2) 2000DEN/KHU
4-Cl	(1) 89.8±1.4	375.7±5.9		
4-Me	(1) 89.9±2.5	376.1±10.5		
4-CF_3	(1) 92.2±1.7	385.8±7.1		
2-tBu	(1) 94.7±1.3	396.2±5.4		
2,2-Me_2	(1) 90.2±1.5	377.4±6.5		

pyrrolidine

$\Delta_f H^o$(R) = 34.1±3 (142.7±12.6)	(1) 90.1±2.4 (2) 87	377±10.0 364.0	PAC	(1) 1997WAY/CLA (2) 2000KRA/CIR

cyclohexalamine, substituted



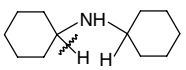
X_1 = H, X_2 = H	94.6	395.9	Correlation	2000DEN/KHU
H, Me	89.8	375.9		
Me, Me	88.1	368.6		

piperidine

$\Delta_f H^o$(R) = 28.6 (119.7)	(1) 89.5 (2) 92.0±2.4 (3) 90.7	374.5 385±10.0 379.6	(1) PAC (2) PAC (3) Correlation	(1) 1993CLA/WAY (2) 1997WAY/CLA (3) 2000DEN/KHU

(continued)

Table 3.6.2 (continued) C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

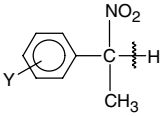
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
morpholine 	(1) 90.8	379.9	PAC	(1) 1993CLA/WAY
	(2) 93.0±2.4	389±10.0		(2) 1997WAY/CLA
	(3) 94	393.3		(3) 1999LAA/MUL
	(4) 92±2	384.9±8.4		(4) 2002LAL/ALL
dicyclohexylamine 	89.6	374.9	Correlation	2000DEN/KHU
methyl isocyanide **H**–CH_2NC $\Delta_f H^o(R)$ = 78.0±2.7 (326.4±11.3)	91.0±2.1	380.7±8.8	Photoelectron	1987MOR/ELL(b)
methanenitrile **H**–CN $\Delta_f H^o(R)$ = 105.5±1.1 (441.4±4.6)	(1) 126.1±0.4	527.6±1.7	(1) Recommend.	(1) 1994BER/ELL
	(2) 126.3±0.2	528.5±0.8	(2) Photolysis	(2) 2000COO/LAN
acetonitrile CH_3**H**$_3$CN $\Delta_f H^o(R)$ = 60.4±1 (252.6±4.2)	(1) 93±2.5	389.1±10.5	(1) Review	(1) 1982MCM/GOL
	(2) 94.8±2.1	396.6±8.8	(2) Photoelectr.	(2) 1987MOR/ELL(b)
	(3) 95.5±1.7	399.6±7.1	(3) PAC	(3) 1989KAM/GRI
	(4) **96**	**401.7**	(4) PAC	(4) 1995WAY/LUS
	(5) 97.0±1	405.8±4.2	(5) Negative ion cycle	(5) 2000LAF/SZA
propanenitrile CH_3CH_2CN $\Delta_f H^o(R)$ = 54.2±2.3 (226.7±12.6)	(1) 89.8±2.3	375.7±9.6	(1) VLPP	(1) 1975KIN/GOD
	(2) **94.0±3**	**393.3±12.6**	(2) Derived from $\Delta_f H^o$ in ref.	(2) 1986PED/NAY
	(3) 90±2	376.6±8.4	(3) AP	(3) 1993HOL/LOS
	(4) 94.9	397.1	(4) Reanal. of pyrolysis data	(4) 1998BRO/BEC

phenylacetonitrile Ph**C**$\mathbf{H}_2$CN	82.3	344.3	AOP	1993BOR/ZHA(b)
pentafluorophenyl acetonitrile C_6F_5**C**$\mathbf{H}_2$CN	83.8	350.6	AOP	1993BOR/ZHA(b)
methae-1,1-dicarbonitrile **C**$\mathbf{H}_2$(CN)$_2$	(1) 90 (2) 87.6	376.6 366.5	(1) AOP (2) Reanal. of pyrolysis data	(1) 1991BOR/CHE (2) 1998BRO/BEC
2-aminoethanenitrile **C**$\mathbf{H}_2$(CN)(NH$_2$)	84.9	355.2	Reanal. of pyrolysis data	1998BRO/BEC
2-methylpropanenitrile (CH$_3$)$_2$C**H**CN $\Delta_f H^o(R)$ = 45.5±3 (190.4±12.6)	(1) 86.5±2.0 (2) 91.9	361.9±8.4 384.5	(1) VLPP (2) Reanal. of pyrolysis data	(1) 1976KIN/GOD (2) 1998BRO/BEC
2-phenyl propanenitrile Ph(Me)C**H**CN	80	334.7	AOP	1988BOR/CHE(b)
diphenylacetonitrile Ph$_2$C**H**CN	(1) 77.5 (2) 76.8	324.3 321.3	AOP	(1) 1988BOR/CHE(b) (2) 1993BOR/ZHA(b)
di(pentafluorophenyl)-acetonitrile (C$_6$F$_5$)$_2$C**H**CN	81.7	341.8	AOP	1993BOR/ZHA(b)
methylmethae-1, 1-dicarbonitrile MeC**H**(CN)$_2$	84.6	354.0	Reanal. of pyrolysis data	1998BRO/BEC
phenylmethane-1, 1-dicarbonitrile PhC**H**(CN)$_2$	77	322.2	AOP	1992ZHA/BOR

(continued)

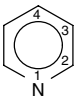
Table 3.6.2 (continued) C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-cyclohexyl-2-phenyl-ethanenitrile c-$C_6H_{11}C\mathbf{H}$(Ph)CN	81	338.9	AOP	1992BOR/ZHA
2-phenyl-propanenitrile MeC**H**(Ph)CN	80	334.7	AOP	1992BOR/ZHA
phenylmethane-1, 1-dicarbonitrile CNC**H**(Ph)CN	77	322.2	AOP	1992BOR/ZHA
2-phenyl-2-(2-pyridyl)-ethanenitrile c-PyNC**H**(Ph)CN	76	318.0	AOP	1992BOR/ZHA
nitromethane $C\mathbf{H}_3NO_2$ $\Delta_f H^o$(R) = 27.5±3.0 (115.1±12.6)	(1) 97.4 (2) 96.3	407.5 402.9	(1) AOP (2) Derived	(1) 1994BOR/SAT (2) 2000MIR/VOR
nitroethane $CH_3C\mathbf{H}_2NO_2$ $\Delta_f H^o$(R) = 14.8±3 (61.9±12.6)	91.4	382.4	AOP	1994BOR/SAT
2-nitropropane $Me_2C\mathbf{H}NO_2$ $\Delta_f H^o$(R) = 1.5±3 (6.3±12.6)	86.8	363.2	AOP	1994BOR/SAT
nitrocyclopropane c-$C_3\mathbf{H}_5NO_2$	88.4	369.9	AOP	1994BOR/SAT

nitrocyclopetane c-$C_5\mathbf{H}_9NO_2$	86.8	363.2	AOP	1994BOR/SAT
nitrocyclohexane c-$C_6\mathbf{H}_{11}NO_2$	88.6	370.7	AOP	1994BOR/SAT
1-phenylnitroethane, substituted  $\Delta_fH^o(R)$ = 40.4±3 (169.0±12.6) Y = H	85.4	357.3	AOP	1995BOR/ZHA(c)
4-F	86.1	360.2		
4-Me	85.6	358.2		
3-MeO	86.9	363.6		
4-MeO	84.9	355.2		
3-NO_2	86.1	360.2		
4-NO_2	86.9	363.6		
3,5-$(NO_2)_2$	88.7	371.1		
nitro(phenylmethoxy) methane $PhCH_2OCH_2NO_2$	86.1	360.2	AOP	1994BOR/SAT
1-aza-1-methyoxy-3-phenyl-2-benzylpro-1-ene $(PhC\mathbf{H}_2)_2C{=}NOMe$	82.9	346.9	AOP	1992ZHA/BOR
pyrrole 				
C-H bond at 2 and 3 site	118.4±1	495.4±4.2	Shock tube	1991MAC/COL

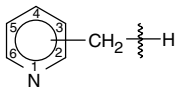
(continued)

Table 3.6.2 (continued) C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$\Delta_f H^o$(pyrrol-2-yl) = 92.2 (385.8)				
$\Delta_f H^o$(pyrrol-3-yl) = 92.2 (385.8)				
pyridine 				
C-H bond at 2 site	(1) **105±0.2**	**439.3±0.8**	Shock tube	(1) 1997KIE/ZHA
	(2) 102.7	429.7		(2) 1992DOU/MAC
at 3 site	(1) 112±2	468.6±8.4		
at 4 site	(1) 112±2	468.6±8.4		
$\Delta_f H^o$(pyrid-2-yl) = 86.5 (361.9)				
$\Delta_f H^o$(pyrid-3-yl) = 93.5 (391.2)				
$\Delta_f H^o$(pyrid-4-yl) = 93.5 (391.2)				
pyrimidine 				
C–H bond at 2 site	(1) 98±2	410.0±8.4	Shock tube	(1) 1997KIE/ZHA
	(2) 95.8	400.8		(2) 1992DOU/MAC
at 4 site	(1) 103±2	431.0±8.4		
	(2) 102.8	430.1		
at 5 site	(1) 112±2	468.6±8.4		
	(2) 111.2	465.3		
$\Delta_f H^o$(pyrimid-2-yl) = 92.7±2 (387.9±8.4)				

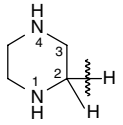
$\Delta_f H^o$(pyrimid-4-yl) = 97.7±2
(408.4±8.4)
$\Delta_f H^o$(pyrimid-5-yl) = 106.7±2
(446.4±8.4)

pyridine, substituted

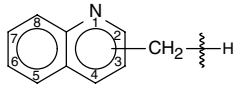


2-CH_3	87.2	365.0	Correlation	2002KRO/TUM
3-CH_3	90.4	378.2		
4-CH_3	86.5	362.1		
2,4,6-$(CH_3)_3$	87.7	366.9		

piperazine	(1) 90 (2) 93	376.6 389.1	(1) PAC (2) PAC, revised	(1) 1993CLA/WAY (2) 1999LAA/MUL



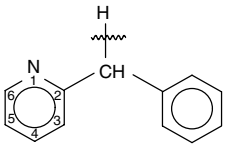
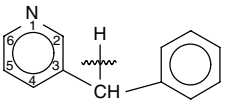
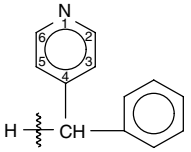
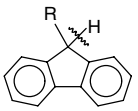
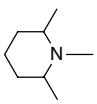
quinline, substituted

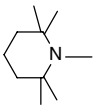
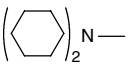


2-CH_3	87.6	366.6	Correlation	2002KRO/TUM
3-CH_3	88.9	372.1		
4-CH_3	86.1	360.1		
5-CH_3	87.5	366.3		
6-CH_3	88.7	371.0		
7-CH_3	88.7	371.0		
8-CH_3	90.3	377.8		

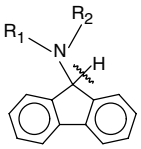
(continued)

Table 3.6.2 (continued) C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-benzyl pyridine 	(1) 82.3 (2) 82	344.3 343.1	(1) VLPP (2) AOP	(1) 1984ROS/MCM (2) 1992ZHA/BOR
3-benzyl pyridine 	84	351.5	AOP	1992ZHA/BOR
4-benzyl pyridine 	(1) 82.3 (2) 83	344.3 347.3	(1) VLPP (2) AOP	(1) 1984ROS/MCM (2) 1992ZHA/BOR
fluorene, substituted 				
R = 	66	276.1	AOP	1992ZHA/BOR(b)
	68	284.5		
	72	301.2		
	71.5	299.2		
	72	301.2		

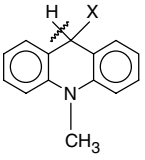
	71	297.1		
	73	305.4		

fluorene, substituted



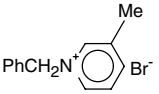
R_1 = Me,	R_2 = Me	71.5	299.2	AOP	1992ZHA/BOR(b)
Et	Et	70.5	295.0		
iPr	iPr	73	305.4		
nBu	Me	72	301.2		
$PhCH_2$	Me	72.5	303.3		

10-methyl-9,
10-dihydro-acridine,
substituted



X = H	72.0±1.6	301.2±6.7	Electronchem.	1998ANN/FRA
CN	71.3±1.5	298.3±6.3		

benzyl trimethylammonium chloride $PhCH_2^+NMe_3\ Cl^-$	90.5	378.7	AOP	1993ZHA/BOR

3-methyl-1-benzylpyridinium bromide 	84.7	354.4	AOP	1993ZHA/BOR

(continued)

Table 3.6.2 (continued) C–H BDEs with α-N, -CN, -NO, -NO_2, and -NN

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-benzyl pyridinium chloride $PhC\mathbf{H}_2^+NPy\ Cl^-$	84.7	354.4	AOP	1993ZHA/BOR
1-acetonitrile trimethyl-ammonium chloride $Me_3^+NC\mathbf{H}_2CN\ Cl^-$	95.3	398.7	AOP	1990BOR/ZHA
1-acetonitrile pyridinium chloride $PyN^+C\mathbf{H}_2CN\ Cl^-$	87.6	366.5	AOP	1990BOR/ZHA

3.6.3 C–H BDEs with α-O, -N and their groups

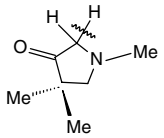
Table 3.6.3 C–H BDEs with α-O, -N and their groups

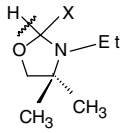
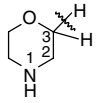
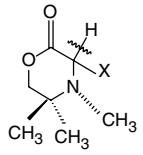
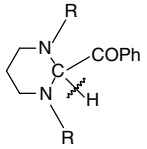
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
(1Z)-2-aza-2-methoxy-1, 1-phenylvinylamine $PhC(NH_2)=NOC\mathbf{H}_3$	94.9	397.1	AOP	1992BOR/JI
2-methoxyethanenitrile $(CN)C\mathbf{H}_2OMe$	90.3	377.8	Reanal. of pyrolysis data	1998BRO/BEC
N,N-dimethylacetamide $Me_2NC(O)C\mathbf{H}_3$	91.0	380.9	Correlation	2000DEN/KHU

methyl 2-(dimethylamino)-acetate $Me_2NC\mathbf{H}_2C(O)Me$	77	322.2	PAC	1993CLA/WAY
N-iso-propylacetamide $(CH_3)_2C\mathbf{H}NHC(O)Me$	93.1	389.5	Correlation	2000DEN/KHU
glycine ion $NH_2C\mathbf{H}_2C(O)O^-$	≤82.0	≤343.0	Electrochem.	1997ZHA/LIN
glycine $NH_2C\mathbf{H}_2C(O)OH$	≤78.6	≤329.0	Electrochem.	1997ZHA/LIN
methyl-2-aminoacetate $NH_2C\mathbf{H}_2C(O)OMe$	84.3	352.7	Reanal. of pyrolysis data	1998BRO/BEC
ethyl 2-aminoacetate $NH_2C\mathbf{H}_2C(O)OEt$	79–83	330.5–347.3	PAC	1993CLA/WAY
ethyl 3-(dimethylamino) prooanoate $Me_2N(C\mathbf{H}_2)_2C(O)OEt$	88.0	368.0	Correlation	2000DEN/KHU
2-(dimethylamino)-1-phenylethan-1-one $N(CH_3)_2C\mathbf{H}_2C(O)Ph$	78.3	327.6	Reanal. of pyrolysis data	1998BRO/BEC
glycine anhydride $NH_2C\mathbf{H}_2C(O)OCH_2NH_2$	81.3±3.6	340±15	PAC	1998JON/WAY
nitro(phenylmethoxy) methane $PhC\mathbf{H}_2OCH_2NO_2$	86.1	402.1	AOP	1994BOR/SAT

(continued)

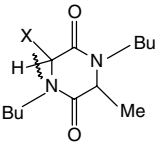
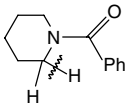
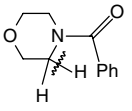
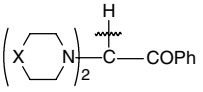
Table 3.6.3 (continued) C–H BDEs with α-O, -N and their groups

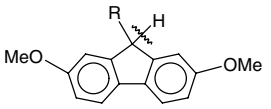
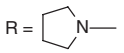
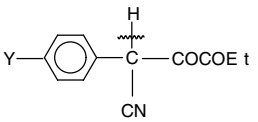
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
tert-butyl-2-aminopropanoate $NH_2C\mathbf{H}MeC(O)OtBu$	81.3	340.2	Reanal. of pyrolysis data	1998BRO/BEC
2-hydroxypropanenitrile $(CN)C\mathbf{H}Me(OH)$	87.3	365.3	Reanal. of pyrolysis data	1998BRO/BEC
alanine anhydride $Me(NH_2)C\mathbf{H}C(O)OCHNH_2Me$	77.7±3.6	325.0±15	PAC	1998JON/WAY
2-methoxy-2-phenylethane-nitrile $MeOC\mathbf{H}(Ph)CN$	77.5	324.3	AOP	1992BOR/ZHA
2-phenyl-2-phenoxyethane-nitrile $PhOC\mathbf{H}(Ph)CN$	79.5	332.6	AOP	1992BOR/ZHA
ethyl 2-cyano-2-phenyl-acetate $C_6H_5C\mathbf{H}(CN)C(O)OEt$	80.9	338.5	AOP	1993BOR/ZHA(b)
ethyl 2-cyano-2-pentafluoro-phenyl-acetate $C_6F_5C\mathbf{H}(CN)C(O)OEt$	85.2	356.5	AOP	1993BOR/ZHA(b)
4,4-dimethyl pyrrolidin-3-one 	78	326.4	PAC	1993CLA/WAY

3-ethyl-4,4-dimethyl-1, 3-oxazolidine 				
X = Me	82.1	343.5	PAC	1993CLA/WAY
C(O)OMe	84.1	351.9		
2-oxomorpholine 	(1) 75 (2) 78	313.8 326.4	(1) PAC (2) PAC, revised	(1) 1993CLA/WAY (2) 1999LAA/MUL
morpholine 	(1) 91 (2) 94	380.7 393.3	(1) PAC (2) PAC, revised	(1) 1993CLA/WAY (2) 1999LAA/MUL
4,5,5-trimethyl morpholin-2-one 				
X = H	75.3	315.1	PAC	1993CLA/WAY
CH_3	77.5	324.3		
phenyl piperazin-2-yl ketone, substituted 				
R = Me	73	305.4	AOP	1992ZHA/BOR(b)
Et	72	301.2		

(continued)

Table 3.6.3 (continued) C–H BDEs with α-O, -N and their groups

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1,4-diazaperhydroine-2, 5-dione, substituted 				
X = H	92.4	386.6	Reanal. of pyrolysis data	1998BRO/BEC
Me	89.4	374.0		
phenyl piperidyl ketone 	94.4	395.0	Correlation	2000DEN/KHU
morpholin-4-yl phenyl ketone 	83.3	348.6	Correlation	2000DEN/KHU
1-phenyl 2, 2-dipiperidylethan-1-one, analogues 				
X = CH_2	74	309.6	AOP	1992ZHA/BOR(b)
O	75	313.8		

fluorene, substituted 				
R = 	69	288.7	AOP	1992ZHA/BOR(b)
ethyl-2-cyano-2-phenylacetate, substituted 				
Y = H	80.3	336.0	AOP	2000CHE/LIU
F	80.3	336.0		
Cl	80.8	338.1		
Me	80.0	334.7		
MeO	78.3	327.6		
$MeCO_2$	82.0	343.1		
CF_3	82.2	343.9		
CN	83.2	348.1		

3.6.4 C–H BDEs with α-C(S), -S, -SO, and -SO_2

Table 3.6.4 C–H BDEs with α-C(S), -S, -SO, and -SO_2

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
thioformaldehyde **H**–C(S)H $\Delta_f H^o$(R) = 71.8±2 (300.4±8.4)	95.5±1.2	399.6±5.0	Recommend.	1994BER/ELL
methanethiol C**H**$_3$SH $\Delta_f H^o$(R) = 36.3±2 (151.9±8.4)	(1) 92.4±2.0 (2) **93.9±2.0**	386.6±8.4 **392.9±8.4**	(1) PIMS (2) Recommend.	(1) 1992RUS/BER (2) 1994BER/ELL

(continued)

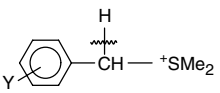
Table 3.6.4 (continued) C–H BDEs with α-C(S), -S, -SO, and -SO_2

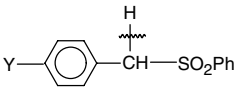
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
dimethyl sulfide $CH_3SC\mathbf{H}_3$ $\Delta_f H^o(R) = 32.7\pm1.4$ (136.8 ± 5.9)	93.7±1.4	392.0±5.9	Resonance fluorescence	1994JEF/NIC
phenyl methyl sulfide $PhSC\mathbf{H}_3$ $\Delta_f H^o(R) = 64.2\pm3$ (268.6 ± 12.6)	93.0	389.1	AOP	1993ZHA/BOR
benzyl phenyl sulfide $PhC\mathbf{H}_2SPh$ $\Delta_f H^o(R) = 104.1\pm3$ (435.6 ± 12.6)	(1) 84.2 (2) 82.2	352.3 343.9	AOP	(1) 1993ZHA/BOR (2) 1998BOR/LIU
di(phenylthio)phenyl methane $(PhS)_2C\mathbf{H}Ph$	81.5	341.0	AOP	1992BOR/ZHA
phenyl diphenylmethyl sulfide $PhSC\mathbf{H}Ph_2$	82.4	344.8	AOP	1992BOR/ZHA
dimethyl sulfoxide $C\mathbf{H}_3SOCH_3$ $\Delta_f H^o(R) = 5.7\pm3$ (23.8 ± 12.6)	94	393.3	AOP	1998BOR/LIU
dimethyl sulfone $C\mathbf{H}_3SO_2CH_3$ $\Delta_f H^o(R) = -42.3\pm3$ (-177.0 ± 12.6)	99	414.2	AOP	1991BOR/HAR

methyl trofluoromethyl sulfone $CH_3SO_2CF_3$	103	431.0	AOP	1991BOR/HAR
methyl phenyl sulfone CH_3SO_2Ph $\Delta_fH^o(R) = -13.7 \pm 3$ (-57.3 ± 12.6)	99	414.2	AOP	1991BOR/HAR
methyl p-NO_2-phenyl sulfone $CH_3SO_2(p\text{-}NO_2\text{–}C_6H_4)$	95	397.5	AOP	1995ZHA/BOR
benzyl methyl sulfone $PhCH_2SO_2Me$ $\Delta_fH^o(R) = -26.1 \pm 3$ (-109.2 ± 12.6)	91	380.7	AOP	1992ZHA/BOR
benzyl trifluoromethyl sulfone $PhCH_2SO_2CF_3$	89	372.4	AOP	1992ZHA/BOR
benzyl tert-butyl sulfone $PhCH_2SO_2tBu$	90	376.6	AOP	1992ZHA/BOR
benzyl phenyl sulfone $PhCH_2SO_2Ph$ $\Delta_fH^o(R) = 1.7 \pm 3$ (7.1 ± 12.6)	(1) 89.7 (2) 90.2	376.3 377.4	AOP	(1) 1998BOR/LIU (2) 1992ZHA/BOR
di(methyl sulfonyl) methane $CH_2(CH_3SO_2)_2$	101.4	424.3	AOP	1994BOR/ZHA
di(trifluoromethyl sulfonyl) methane $CH_2(CF_3SO_2)_2$	113	472.8	AOP	1991BOR/HAR

(continued)

Table 3.6.4 (continued) C–H BDEs with α-C(S), -S, -SO, and -SO_2

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
di(ethyl sulfonyl) methane $C\mathbf{H}_2(EtSO_2)_2$	101.3	423.8	AOP	1994BOR/ZHA
di(isopropyl sulfonyl) methane $C\mathbf{H}_2(iPrSO_2)_2$	100.1	418.8	AOP	1994BOR/ZHA
di(t-butyl sulfonyl) methane $C\mathbf{H}_2(tBuSO_2)_2$	99.7	417.1	AOP	1994BOR/ZHA
di(phenyl sulfonyl) methane $C\mathbf{H}_2(PhSO_2)_2$	98	410.0	AOP	1994BOR/ZHA
((diphenylmethyl) sulfonyl)-benzene $Ph_2C\mathbf{H}SO_2Ph$ $\Delta_f H^o(R) = 24.4 \pm 3$ (–102.1±12.6)	87.3	365.3	AOP	1991BOR/ZHA
di(phenylthio) methane $C\mathbf{H}_2(SPh)_2$	89	372.4	AOP	1995ALN/ZHA
benzyl dibutylsulfonium $PhCH_2{}^{\pm}S(nBu)_2$	83.8	350.6	AOP	1998CHE/LIU
benzyl dibutylsulfonium, substituted 				

Y = H	(2) 83.1	347.7	AOP	(1) 1998CHE/LIU
p-Me	(2) 82.5	345.2		(2) 2000CHE/LIU
p-CN	(2) 86.0	359.8		
p-MeO	(1) 84.6	354.0		
p-MCO_2	(2) 92.0	384.9		
phenyl phenylsulfonyl methane, substituted 				
Y = H	90.3	377.8	AOP	1998BOR/LIU
Me	89.1	372.8		
Cl	91.8	384.1		
Br	90.4	378.2		

3.6.5 C–H BDEs with other heteroatoms at α-position

Table 3.6.5 C–H BDEs with other Heteroatoms at α-Position

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,2-dimethyl-2-silapropane **H**–CH_2SiMe_3 $\Delta_f H^o$(R) = –7.6±1.5 (–32±6)	100±1.5	418	Iodination	1999WAL
2,2,3, 3-tetramethyl-2-silabutane **H**–$CH_2C(CH_3)_2SiMe_3$ $\Delta_f H^o$(R) = –29.8 (–125)	97.8±1.2	409±5	Iodination	1999WAL
alkyldioxaborolanes **H**–$CH_2B(RO)_2$	98.6	412.5	EPR	2000WAL/MCC

chapter four

Tabulated BDEs of C–C bonds

4.1 Saturated hydrocarbons

Table 4.1 C–C BDEs in Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
ethane **CH_3**–CH_3	90.2±0.2	377.4±0.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propane **CH_3**–C_2H_5	88.5±0.5	370.3±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butane **CH_3**–nC_3H_7	88.9±0.7	372.0±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
isobutane **CH_3**–iC_3H_7	88.2±0.9	369.0±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentane **CH_3**–nC_4H_9	88.8±0.7	371.5±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methylbutane **CH_3**–iC_4H_9	88.5±1.1	370.3±4.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.1 (continued) C–C BDEs in Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-methylbutane **CH_3**–sC_4H_9	88.0±0.7	368.2±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethylpropane **CH_3**–tC_4H_9	86.9±0.7	363.6±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpentane **CH_3**–$CH(CH_3)C_3H_7$	88.9±1.0	372.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methylpentane **CH_3**–$CH(C_2H_5)_2$	87.4±1.0	365.7±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butane **C_2H_5**–C_2H_5	86.8±0.6	363.2±2.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentane **C_2H_5**–nC_3H_7	87.3±0.7	365.3±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
isopentane **C_2H_5**–iC_3H_7	86.1±0.9	360.2±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
hexane **C_2H_5**–nC_4H_9	86.9±0.8	363.6±3.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpentane **C_2H_5**–iC_4H_9	86.9±1.3	363.6±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methylpentane **C_2H_5**–sC_4H_9	85.7±0.8	358.6±3.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

2,2-dimethylbutane $\mathbf{C_2H_5}$–tC_4H_9	84.5±0.9	353.5±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpentane $\mathbf{C_3H_7}$–iC_3H_7	86.6±1.3	362.3±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
hexane $\mathbf{nC_3H_7}$–nC_3H_7	87.5±0.8	366.1±3.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpentane $\mathbf{nC_3H_7}$–iC_3H_7	86.6±1.0	362.3±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
heptane $\mathbf{nC_3H_7}$–nC_4H_9	87.3±0.9	365.3±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylhexane $\mathbf{nC_3H_7}$–iC_4H_9	84.2±1.3	352.3±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methylhexane $\mathbf{nC_3H_7}$–sC_4H_9	85.7±0.9	358.6±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethylpentane $\mathbf{nC_3H_7}$–tC_4H_9	84.6±1.0	354.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,3-dimethylbutane $\mathbf{iC_3H_7}$–iC_3H_7	84.5±1.1	353.5±4.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylhexane $\mathbf{iC_3H_7}$–nC_4H_9	86.1±1.1	360.2±4.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,4-dimethylpentane $\mathbf{iC_3H_7}$–iC_4H_9	85.9±1.3	359.4±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.1 (continued) C–C BDEs in Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,3-dimethylpentane **iC$_3$H$_7$**–sC$_4$H$_9$	84.7±1.0	354.4±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2,3-trimethylbutane **iC$_3$H$_7$**–tC$_4$H$_9$	81.5±1.1	341.0±4.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
octane **nC$_4$H$_9$**–nC$_4$H$_9$	87.0±0.9	364.0±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylheptane **nC$_4$H$_9$**–iC$_4$H$_9$	86.8±1.3	363.2±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methylheptane **nC$_4$H$_9$**–sC$_4$H$_9$	85.6±0.9	358.2±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethylhexane **nC$_4$H$_9$**–tC$_4$H$_9$	83.9±1.0	351.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,5-dimethylhexane **iC$_4$H$_9$**–iC$_4$H$_9$	86.6±1.5	362.3±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,4-dimethylhexane **iC$_4$H$_9$**–sC$_4$H$_9$	85.3±1.3	356.9±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,3,4-trimethylpentane **iC$_4$H$_9$**–tC$_4$H$_9$	81.3±1.3	340.3±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3,4-dimethylhexane **sC$_4$H$_9$**–sC$_4$H$_9$	83.3±0.8	348.5±3.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

2,2,3-trimethylpentane **s-C$_4$H$_9$**–tC$_4$H$_9$	80.4±1.0	336.4±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2,3,3-tetramethylbutane **tC$_4$H$_9$**–tC$_4$H$_9$	77.1±1.0	322.6±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,3-trimethylpentane **iC$_3$H$_7$**–C(CH$_3$)$_2$C$_2$H$_5$	79.7±1.5	333.5±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
nonane **nC$_4$H$_9$**–nC$_5$H$_{11}$	86.1±2.0	360.2±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethylheptane **nC$_4$H$_9$**–neoC$_5$H$_{11}$	81.8±2.0	342.3±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
2,2,5-trimethylhexane **iC$_4$H$_9$**–neoC$_5$H$_{11}$	85.9±2.0	359.4±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
2,2,3,3,-tetramethylpentane **tC$_4$H$_9$**–C(CH$_3$)$_2$C$_2$H$_5$	75.3±1.5	315.1±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2,4,4-tetramethypentane **tC$_4$H$_9$**–neoC$_5$H$_{11}$	78±2.2	326.4±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylnonane **nC$_6$H$_{13}$**–iC$_4$H$_9$	86.8±2.0	363.2±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
5-methylnonane **nC$_4$H$_9$**–CH(CH$_3$)(nC$_4$H$_9$)	87.4±2.0	365.7±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dodecane **nC$_6$H$_{13}$**–nC$_6$H$_{13}$	85.0±2.0	355.6±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.1 (continued) C–C BDEs in Saturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
methylcyclopentane **CH_3**–c-C_5H_9	85.6±1.2	358.2±5.0	Derived from Δ_fH^o in ref.	1986PED/NAY
methylcyclohexane **CH_3**–c-C_6H_{11}	90.1±1.8	377.0±7.5	Derived from Δ_fH^o in ref.	1986PED/NAY
ethylcyclobutane **C_2H_5**–c-C_4H_7	86.1±1.3	360.2±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
ethylcyclopentane **C_2H_5**–c-C_5H_9	84.0±1.3	351.5±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
ethylcyclohexane **C_2H_5**–c-C_6H_{11}	87.4±1.3	365.7±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
propylcyclopentane **nC_3H_7**–c-C_5H_9	84.4±1.3	353.1±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
propylcyclohexane **nC_3H_7**–c-C_6H_{11}	87.8±2.0	367.4±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
butylcyclohexane **nC_4H_9**–c-C_6H_{11}	85.3±1.5	356.9±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
cyclohexaxylcyclohexane **c-C_6H_{11}**–c-C_6H_{11}	88.2±2.0	369.0±8.4	Derived from Δ_fH^o in ref.	1988LIA/BAR

1-adamantylmethane 1-adamantyl-**CH_3**	(1) 84.3±3	352.7±12.6	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1988LIA/BAR
	(2) 82.5	345.2	(2) Derived	(2) 2001MAT/LEB
2-adamantylmethane 2-adamantyl-**CH_3**	90.5±3	378.7±12.6	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR

4.2 *Chain unsaturated hydrocarbons*

Table 4.2 C–C BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
acetylene **CH**≡CH	229.5±1.0	960.2±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethylene **CH_2**=CH_2	174.1±1.5	728.4±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propyne **CH_3**–C≡CH	126.0±1.0	527.2±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-butyne **C_2H_5**–C≡CH	124.0±1.0	518.8±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-butyne **CH_3**–CH_2C≡CH	(1) 76.0±2 (2) **76.6±1.2**	318.0±8.4 **320.5±5.0**	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1978KIN (2) 1986PED/NAY
2-butyne **CH_3**–C≡CCH	121.3±3.2	507.5±13.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-pentyne **CH_3**–CH_2C≡CCH_3	73.7±1.5	308.4±6.3	VLPP	1982NGU/KIN

(continued)

Table 4.2 (continued) C–C BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-methy-1-butyne **CH_3**–CH(CH_3)C≡CH	73±2	305.4±8.4	VLPP	1981NGU/KIN
2-methy-1-pentyne **CH_3**–CH(CH_3)C≡CCH_3	76.7±1.5	320.9±6.3	VLPP	1981KIN/NGU
2,2-dimethy-1-butyne **CH_3**–C(CH_3)$_2$C≡CH	70.7±1.5	295.8±6.3	VLPP	1977KIN
2,2-dimethy-1-pentyne **CH_3**–C(CH_3)$_2$C≡CCH_3	72.5±1.5	303.3±6.3	VLPP	1981KIN/NGU
1-hexyne **nC_3H_7**–CH_2C≡CH	73.2±1.5	306.3±6.3	VLPP	1981KIN
2-ethyl-1-pentyne **sC_4H_9**–CH_2C≡CH	71.7±1.5	300.0±6.3	SPTS	1978TSA
1,2-butadiene **CH_3**–CH=CCH_2	86.0±1.4	359.8±5.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,3-butadiene **C_2H_3**–CH=CH_2	116.9±1.5	489.1±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-methylcyclopropene **CH_3**-cyclopro-en-1-yl	81.4±5	340.6±20.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

1-butene **CH_3**–$CH_2CH=CH_2$	(1) 76.5±2.2 (2) **75.9±0.9**	320.1±9.2 **317.6±3.8**	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1981NGU/KIN (2) 1986PED/NAY
1-butene **C_2H_5**–$CH=CH_2$	100.0±1.0	418.4±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(E)-2-butene (E)-**CH_3**–$CH=CHCH_3$	101.6±2.0	425.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-2-butene (Z)-**CH_3**–$CH=CHCH_3$	102.6±2.0	429.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,2-pentadiene **C_2H_5**–$CH=C=CH_2$	80.6±1.5	337.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,4-pentadiene **C_2H_3**–$CH_2CH=CH_2$	87.2±1.2	364.8±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(E)-1,3-pentadiene (E)-**CH_2=CH**–$CH=CHCH_3$	117.2±2.0	490.4±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-1,3-pentadiene (Z)-**CH_2=CH**–$CH=CHCH_3$	118.5±2.0	495.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-pentene **C_2H_5**–$CH_2CH=CH_2$	74.3±1.5	310.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(E)-2-pentene (E)-**CH_3**–$CH_2CH=CHCH_3$	77.6±2.2	324.7±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-2-pentene (Z)-**CH_3**–$CH_2CH=CHCH_3$	78.6±2.2	328.9±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.2 (continued) C–C BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-pentene **C_2H_5**–CH=CHCH_3	99.8±2.0	417.6±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
2-methyl-1-butene **CH_3**–$CH_2C(CH_3)$=CH_2	(1) 72.0±2 (2) **74.1±1.0**	301.2±8.4 **310.0±4.2**	(1) Kinetics (2) Derived from Δ_fH^o in ref.	(1) 1981STE/ROW (2) 1986PED/NAY
3-methyl-1-butene **CH_3**–$CH(CH_3)$CH=CH_2	72.3±1.5	302.5±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
3,3-dimethyl-1-butene **CH_3**–$C(CH_3)_2$CH=CH_2	(1) 68.1±1.5 (2) **67.5±1.5**	284.9±6.3 **282.4±6.3**	(1) Derived (2) Derived from Δ_fH^o in ref.	(1) 1982MCM/GOL (2) 1986PED/NAY
3-methyl-1-butene **iC_3H_7**–CH=CH_2	99.2±1.5	415.1±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
1,5-hexadiene **C_3H_5**–C_3H_5	61.5±1.0	257.3±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
1-hexene **nC_3H_7**–CH_2CH=CH_2	(1) 70.7±2 (2) **75.0±1.0**	295.8±8.4 **313.8±4.2**	(1) SPST (2) Derived from Δ_fH^o in ref.	(1) 1976TSA (2) 1986PED/NAY
1-hexene **nC_4H_9**–CH=CH_2	100.6±1.3	420.9±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
(E)-2-hexene (E)-**C_2H_5**–CH_2CH=CHCH_3	76.2±2.4	318.8±10.0	Derived from Δ_fH^o in ref.	1986PED/NAY

(Z)-2-hexene (Z)-$\mathbf{C_2H_5}$–$CH_2CH{=}CHCH_3$	76.6±2.4	320.5±10.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-hexene $\mathbf{C_3H_7}$–$CH{=}CHCH_3$	100.5±2.0	420.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-1-pentene $\mathbf{C_2H_5}$–$CH_2C(CH_3){=}CH_2$	73.2±1.0	306.3±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methyl-1-pentene $\mathbf{C_2H_5}$–$CH(CH_3)CH{=}CH_2$	70.8±1.5	296.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methyl-1-pentene $\mathbf{sC_4H_9}$–$CH{=}CH_2$	99.6±1.0	416.6±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
4-methyl-1-pentene $\mathbf{iC_3H_7}$–$CH_2CH{=}CH_2$	74.1±1.0	310.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
4-methyl-1-pentene $\mathbf{iC_4H_9}$–$CH{=}CH_2$	100.6±1.5	420.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(E)-4-methyl-2-pentene (E)-$\mathbf{iC_3H_7}$–$CH{=}CHCH_3$	99.5±2.0	416.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-4-methyl-2-pentene (Z)-$\mathbf{iC_3H_7}$–$CH{=}CHCH_3$	100.5±2.0	420.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3,3-dimethyl-1-butene $\mathbf{tC_4H_9}$–$CH{=}CH_2$	97.7±1.3	408.8±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-heptene $\mathbf{nC_4H_9}$–$CH_2CH{=}CH_2$	74.3±1.0	310.9±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

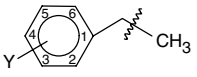
(continued)

Table 4.2 (continued) C–C BDEs in Chain Unsaturated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
5-methyl-1-hexene **iC_4H_9**–$CH_2CH{=}CH_2$	73.2±1.5	306.3±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
5-methyl-1-hexene **nC_3H_7**–$CH_2C(CH_3){=}CH_2$	70.1±1.6	293.3±6.7	Derived from Δ_fH^o in ref.	1986PED/NAY
2,4-dimethyl-1-pentene **iC_3H_7**–$CH_2C(CH_3){=}CH_2$	71.6±1.5	299.6±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
4,4-dimethyl-1-pentene **tC_4H_9**–$CH_2CH{=}CH_2$	71.9±1.5	300.8±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
(E)-4,4-dimethyl-2-pentene (E)-**tC_4H_9**–$CH{=}CHCH_3$	96.6±2.0	404.2±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
(Z)-4,4-dimethyl-2-pentene (Z)-**tC_4H_9**–$CH{=}CHCH_3$	100.5±2.0	420.5±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
2,4,4-trimethyl-1-pentene **tC_4H_9**–$CH_2C(CH_3){=}CH_2$	68.6±2.0	287.0±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
1-octene **nC_5H_{11}**–$CH_2CH{=}CH_2$	73.3±1.5	306.7±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
3-cyclopentylpropene **c-pentyl**-CH_2CHCH_2	71.9±1.5	300.8±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
vinylcyclohexane **c-hexayl**-$CHCH_2$	91.3±2.0	382.0±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY

4.3 *Aromatic hydrocarbons*

Table 4.3 C–C BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
methylbenzene **CH_3**–C_6H_5	102.0±1.0	426.8±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
vinylbenzene **C_2H_3**–C_6H_5	115.2±1.3	482.0±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethylbenzene, substituted  				
Y = H	(1) 74.1 (2) 75.8±1.0 (3) **76.4±1.7**	310.0 317.1 **319.7±7.1**	(1) VLPP (2) Derived (3) Derived from $\Delta_f H^o$ in ref.	(1) 1980BAR/STE (2) 1982MCM/GOL (3) 1986PED/NAY
2-Me	(1) 72.9	305.0		
3-Me	(1) 73.8	308.8		
4-CH_2=CH	(4) 70.6	295.4	(4) VLPP	(4) 1986ROB/STE
2,6-Me_2	(1) 71.2	297.9		
3,6-Me_2	(1) 72.5	303.8		
3,5-Me_2	(1) 73.5	307.5		
ethylbenzene **C_2H_5**–C_6H_5	100.2±1.0	419.2±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclopropylbenzene **c-C_3H_5**–C_6H_5	109.8±1.2	459.4±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

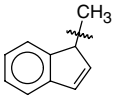
Table 4.3 (continued) C–C BDEs in Aromatic Hydrocarbons

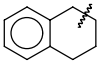
The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
prop-2-enylbenzene $\mathbf{C_2H_3}$–$CH_2C_6H_5$	87.9	367.8	Derived from Δ_fH^o in ref.	1999VER(c)
propylbenzene $\mathbf{C_2H_5}$–$CH_2C_6H_5$	74.9±1.7	313.4	Derived from Δ_fH^o in ref.	1986PED/NAY
propylbenzene $\mathbf{nC_3H_7}$–C_6H_5	100.8±1.0	421.7±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
iso-propylbenzene $\mathbf{CH_3}$–$CH(CH_3)C_6H_5$	(1) 73.8 (2) **74.6±1.5**	308.8 **312.1±6.3**	(1) VLPP (2) Recal.	(1) 1981ROB/STE (2) 1984ROS/MCM
iso-propylbenzene $\mathbf{iC_3H_7}$–C_6H_5	98.9±1.2	413.8±5.0	Derived from Δ_fH^o in ref.	1986PED/NAY
butylbenzene $\mathbf{nC_4H_9}$–C_6H_5	100.6±1.0	420.9±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
butylbenzene $\mathbf{nC_3H_7}$–$CH_2C_6H_5$	75.3±1.7	315.1±7.1	Derived from Δ_fH^o in ref.	1986PED/NAY
4-phenyl-1-butene $\mathbf{CH_2{=}CHCH_2}$–$CH_2C_6H_5$	61.4±2	256.9±8.4	VLPP	1979KIN/NGU
2-methyl-1-phenylpropane $\mathbf{iC_3H_7}$–$CH_2C_6H_5$	74.5±1.7	311.7±7.1	Derived from Δ_fH^o in ref.	1986PED/NAY
2-methylpropylbenzene $\mathbf{iC_4H_9}$–C_6H_5	100.7±1.5	421.3±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY

4-phenyl-1-butyne $\mathbf{C_6H_5CH_2}$–$CH_2C{\equiv}CH$	61.4±2	256.9±8.4	VLPP	1979KIN/NGU
2-phenyl-propane $\mathbf{CH_3}$–$CH(CH_3)C_6H_5$	74.6±1.5	312.1±6.3	VLPP	1981ROB/STE
2-phenylbutane $\mathbf{C_2H_5}$–$CH(CH_3)C_6H_5$	73.7±1.5	308.4±6.3	VLPP	1981ROB/STE
tert-butylbenzene $\mathbf{CH_3}$–$C(CH_3)_2C_6H_5$	72.5±2.0	303.3±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
((1Z)-prop-1-enyl)benzene $\mathbf{CH_3}$–$CH_2CHCHPh$	70.6	295.4	VLPP	1986ROB/STE
1,1-diphenylethane $\mathbf{CH_3}$–$CH(C_6H_5)_2$	71.3	298.3	VLPP	1984ROS/MCM
2,2-diphenylpropane $\mathbf{CH_3}$–$C(CH_3)(C_6H_5)_2$	69.5±2	290.8±8.4	VLPP	1981STE
biphenyl $\mathbf{C_6H_5}$–C_6H_5	114.4±1.5	478.6±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
diphenylmethane $\mathbf{C_6H_5}$–$CH_2C_6H_5$	90.4±2.0	378.2±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
bibenzyl $\mathbf{C_6H_5CH_2}$–$CH_2C_6H_5$	62.6±2.2	261.9±9.2	Derived from Δ_fH^o in ref.	1986PED/NAY
triphenylmethane $\mathbf{C_6H_5}$–$CH(C_6H_5)_2$	86.3±2.0	361.1±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY

(continued)

Table 4.3 (continued) C–C BDEs in Aromatic Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
tetraphenylmethane $\mathbf{C_6H_5}$–$C(C_6H_5)_3$	77.5±3	324.3±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,1,2,2-tetraphenylethane $\mathbf{Ph_2CH}$–$CHPh_2$	59.1±2	247.3±8.4	Derived from $\Delta_f H^o$ in ref.	1990BEC/DOG
1,2,2,2-tetraphenylethane $\mathbf{PhCH_2}$–CPh_3	54.8±3.5	229.3±14.6	Derived from $\Delta_f H^o$ in ref.	1990BEC/DOG
1-methylindene 	72.4	302.9	VLPP	1986ROB/STE
1-methylnaphthalene $\mathbf{CH_3}$-naphth-1-yl	103.8±2.0	434.3±8.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
2-methylnaphthalene $\mathbf{CH_3}$-naphth-2-yl	105.3±2.0	440.6±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclohexylbenzene $\mathbf{c\text{-}C_6H_{11}}$–$C_6H_5$	98.7±2.0	413.0±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl-1-naphthalene $\mathbf{CH_3}$-1-naphthymethyl	72.9±1.5	305.0±6.3	VLPP	1980MCM/TRE
ethyl-9-anthracene $\mathbf{CH_3}$-9-anthracenylmethyl	67.6±1.5	282.8±6.3	VLPP	1980MCM/TRE

ethyl-9-phenanthrene **CH_3**-9-phenanthrenylmethyl	72.9±1.5	305.0±6.3	VLPP	1980MCM/TRE
cyclohexene 	74.8	313.0	Derived	1997DOR/PUG
tetralin 	72.9	305.0	SPST	1994TSA/CUI

4.4 *Halogenated hydrocarbons*

Table 4.4 C–C BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
tetrafluoroethylene **CF_2**=CF_2	(1) 76.3	319.2	(1) Pyrolysis, MS detect.	(1) 1968ZMB/UY
	(2) 68.7	287.4	(2) Derived from $\Delta_f H^o$ in ref.	(2) 2002CRC
tetrachloroethylene **CCl_2**=CCl_2	110.6	462.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
perfluoroethane **CF_3**–CF_3	(1) 93±2	389.1±8.4	(1) Pyrolysis	(1) 1965TSC
	(2) **98.7±2.5**	**413.0±10.5**	(2) Kinetics	(2) 1967COO/WHI
	(3) 96.4±5.2	403.3±21.8	(3) Review	(3) 2001LAZ/PRO
pentafluoroethane **CF_3**–CHF_2	95.5±2	399.6±8.4	Derived from $\Delta_f H^o$ in ref.	1975CHE/ROD

(continued)

Table 4.4 (continued) C–C BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
chloropentafluoroethane **CF_3**–$CClF_2$	89.3±3	373.6±12.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,1,1,2-tetrafluoroethane **CF_3**–CH_2F	95±2	397.5±8.4	Derived from $\Delta_f H^o$ in ref.	1975CHE/ROD
1-bromo-1-chloro-2,2,2-trifluoroethane **CF_3**–CHBrCl	90.4±2.5	378.2±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-bromo-2,2,2-trifluoroethane **CF_3**–CH_2Br	95.0±2	397.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,1,1-trifluoro-2-iodoethane **CF_3**–CH_2I	97.6±2.5	408.4±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,1,1-trifluoroethane **CF_3**–CH_3	101.2±1.1	423.4±4.6	Kinetics	1973ROD/FOR
1,1,2,2-tetrafluoroethane **CHF_2**–CHF_2	91.4±3.7	382.4±15.5	SPST	1971MIL/HAR
1,2-dichlorotetrafluoroethane **$CClF_2$**–$CClF_2$	90.5±3	378.7±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,1,2-trifluoroethane **CHF_2**–CH_2F	94.2±4	394.1±16.7	Derived from $\Delta_f H^o$ in ref.	1968LAC/SKI

1,2-difluoroethane **CH_2F**–CH_2F	88±2	368.2±8.4	Thermal elimination	1971KER/TIM
1,1-difluoroethane **CHF_2**–CH_3	96.8±2	405.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
fluoroethane **CH_2F**–CH_3	(1) 90.4±3 (2) **93.2±2**	378.2±12.6 **389.9±8.4**	(1) Derived from $\Delta_f H^o$ in ref. (2) Derived from $\Delta_f H^o$ in ref.	(1) 1975CHE/ROD (2) 1998SMI
1-chloro-1-fluoroethane **CHClF**–CH_3	95.5±3	399.6±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
perfluoropronene **CF_3**–$CF=CF_2$	85±2.5	355.6±10.5	SPST	1995HE
perchloroethane **CCl_3**–CCl_3	(1) 70.1±3.5 (2) **68.3±1.5**	293.3±14.6 **285.8±6.3**	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,1,2-tetrachloro-2, 2-difluoroethane **CCl_3**–$CClF_2$	67.4±3	282.0±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
pentachloroethane **CCl_3**–$CHCl_2$	(1) 75.4±3.9 (2) **73.2±2**	315.5±16.3 **306.3±8.4**	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,1,2-tetrachloroethane **CCl_3**–CH_2Cl	(1) 82.3±3 (2) **77.4±2**	344.3±12.6 **323.8±8.4**	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1997CIO/LIU (2) 1998NIST

(continued)

Table 4.4 (continued) C–C BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1,1,1-trichloroethane **CCl_3**–CH_3	(1) 87.6±2.0 (2) **86.6±1.5**	366.5±8.4 **362.3±6.3**	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,2,2-tetrachloroethane **$CHCl_2$**–$CHCl_2$	(1) 84.0±4.7 (2) **80.3±2**	351.5±19.7 336.0±8.4	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,2-trichloroethane **$CHCl_2$**–CH_2Cl	86.5±4.0	361.9±16.7	Derived	1997CIO/LIU
1,1-dichloroethane **$CHCl_2$**–CH_3	(1) 89.8±3.3 (2) **87.3±0.8**	375.7±13.8 **365.1±3.3**	Derived	(1) 1997CIO/LIU (2) 1998SEE
1,1-bromochloroethane **CHBrCl**–CH_3	91.9	384.5	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
1,2-dibromo-1, 2-dichloro-ethane **CHClBr**–CHClBr	82.4±3	344.8±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,2-dichloroethane **CH_2Cl**–CH_2Cl	(1) 87.2±3.3 (2) **86.2±2.0** (3) 87.1±1.3	364.8±13.8 **360.7±8.4** 364.6±5.3	(1) Derived (2) Derived from $\Delta_f H^o$ in ref. (3) Derived	(1) 1997CIO/LIU (2) 2002CRC (3) 2002LAG/DIO
1,1-dibromoethane **$CHBr_2$**–CH_3	89.1	372.8	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
1-bromo-2-chloroethane **CH_2Br**–CH_2Cl	89.4	374.0	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR

1,2-dibromoethane **CH_2Br**–CH_2Br	89.8±2	375.7±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,2-diiodoethane **CH_2I**–CH_2I	92.5±2.5	387.0±10.5	Derived from $\Delta_f H^o$ in ref.	1994CAR/LAY
chloroethane **CH_3**–CH_2Cl	89.8±2.2	375.7±9.2	Derived	1997CIO/LIU
bromoethane **CH_3**–CH_2Br	90.3±2	377.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iodoethane **CH_3**–CH_2I	91.9±2	384.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
perfluoropropane **CF_3**–CF_2CF_3	101.4±3	424.3±13.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
3,3,3-trifluoroprop-1-yne **CF_3**–C≡CH	122.7	513.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
3,3,3-trifluoropropene **CF_3**–CH=CH_2	107±3	447.7±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
fluoropropane **CH_3**–CH_2CH_2F	91.6±3	383.3±12.6	Derived from $\Delta_f H^o$ in ref.	1998SMI
fluoropropane **CH_3CH_2**–CH_2F	101.5±3	424.7±12.6	Derived from $\Delta_f H^o$ in ref.	1998SMI
1-chloropropane **CH_3**–CH_2CH_2Cl	88.8±0.6	371.4±2.8	Derived	1998SEE

(continued)

Table 4.4 (continued) C–C BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-chloropropane **CH_3**–$CHClCH_3$	87.8±0.5	367.5±2.0	Derived	1998SEE
1,2-dichloropropane **CH_2Cl**–$CHClCH_3$	85.2±2.0	356.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,3-dichloropropane **CH_2Cl**–CH_2CClH_2	88.2±2	369.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2,2-dichlororopane **CH_3**–CCl_2CH_3	86.7±2	362.8±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,2-dibromopropane **CH_2Br**–$CHBrCH_3$	87.8±2	367.4±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,3-dichlorobutane **CH_2ClCH_2**–$CHClCH_3$	87.1±2	364.4±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,4-dichlorobutane **CH_2ClCH_2**–CH_2CClCH_2	88.2±2	369.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2,3-dibromobutane **CH_3CHBr**–$CHBrCH_3$	85.0±2	355.6±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-bromobutane **CH_2Br**–C_3H_7	89.8±2	375.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-bromobutane **CH_3CHBr**–C_2H_5	87.5±2	366.1±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC

1-chlorobutane **CH_2Cl**–C_3H_7	88.7±2	371.1±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chlorobutane **CH_3CHCl**–C_2H_5	85.2±2	356.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-chlorobutane **CH_2Cl**–iC_3H_7	87.1±2	364.4±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-bromopentane **CH_2Br**–nC_4H_9	89.8±2	375.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-chloropentane **CH_2Cl**–nC_4H_9	88.4±2	369.9±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-chloropentane **CH_2ClCH_2**–C_3H_7	87.8±2	367.4±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chloro-3-methyl-butane **CH_2Cl**–iC_4H_9	87.6±2	366.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chloro-3-methyl-butane **CH_2ClCH_2**–iC_3H_7	86.1±2	360.2±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-bromohexane **CH_2Cl**–nC_5H_{11}	88.8±2	371.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chlorohexane **CH_2ClCH_2**–nC_4H_9	85.7±2	358.6±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
fluorononane **CH_2FCH_2**–nC_7H_{13}	90.0±3	376.6±12.6	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER

(continued)

Table 4.4 (continued) C–C BDEs in Halogenated Hydrocarbons

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,2-difluorononane **CH_3CF_2**–nC_7H_{13}	91.2±3	381.6±12.6	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
(chloromethyl)benzene **CH_2Cl**–C_6H_5	102.7	429.7	Derived from $\Delta_f H^o$ in ref.	2002VER/KRA
(bromomethyl)benzene **CH_2Br**–C_6H_5	100.3	419.7	Derived from $\Delta_f H^o$ in ref.	2002VER/KRA
(iodomethyl)benzene **CH_2I**–C_6H_5	103.4	432.6	Derived from $\Delta_f H^o$ in ref.	2002VER/KRA
(trifluoromethyl)benzene **CF_3**–C_6H_5	110.7±3	463.2±12.6	Derived from $\Delta_f H^o$ in ref.	1994PED
pentafluorophenylmethane **CH_3**–C_6F_5	105.0	439.3	Derived	1975CHO/GOL
pentafluorophenyl trifluoromethane **CF_3**–C_6F_5	104.0	435.1	Derived	1975CHO/GOL
(2,2,2-trifluoroethyl)benzene **CF_3**–$CH_2C_6H_5$	86.1±3	360.2±12.6	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
(3,3-difluoropropyl)benzene **CHF_2**–$CH_2CH_2C_6H_5$	97.8±4	409.2±16.7	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER

(3,3-difluoropropyl)benzene **CHF_2CH_2**–$CH_2C_6H_5$	79.1±3	331.0	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
bipentafluorophenyl **C_6F_5**–C_6F_5	116.7	488.3	Combustion	1979PRI/SAP
(2,2,2-trifluoro-1-phenyl-ethyl)benzene **CF_3**–$CHPh_2$	84.2±4	352.3±16.7	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
(2,2,2-trifluoro-1, 1-diphenyl-ethyl)benzene **CF_3**–CPh_3	69.5±4	290.8±16.7	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
(3-fluoro-1, 1-diphenyl-propyl)benzene **CH_2FCH_2**–CPh_3	65.7±4	279.1±16.7	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
(3,3-difluoro-1, 1-diphenyl-propyl)benzene **CHF_2CH_2**–CPh_3	63.1±4	264.0±16.7	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER

4.5 Organic compounds containing heteroatoms

4.5.1 Organic compounds containing oxygen atoms

Table 4.5.1 C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
ethanol **CH_3**–CH_2OH	87.2±1.0	364.8±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2,2-trifluoroethanol **CF_3**–CH_2OH	96.9±1.5	405.4±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC

(continued)

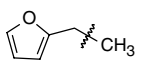
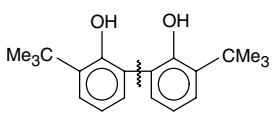
Table 4.5.1 (continued) C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-propanol **C_2H_5**–CH_2OH	85.3±1.2	356.9±5.0	Derived from Δ_fH^o in ref.	1986PED/NAY
2,2,3,3-tetrafluoro-1-propanol **CHF_2CF_2**–CH_2OH	90.7±2	379.5±8.4	Derived from Δ_fH^o in ref.	2002CRC
1-butanol **C_3H_7**–CH_2OH	85.4±0.8	357.3±3.3	Derived from Δ_fH^o in ref.	1986PED/NAY
2-methyl-1-propanol **iC_3H_7**–CH_2OH	84.8±1.0	354.8±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
1-pentanol **C_4H_9**–CH_2OH	85.0±1.0	355.6±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
2-methyl-1-butanol **sC_4H_9**–CH_2OH	84.3±1.0	352.7±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
3-methyl-1-butanol **iC_4H_9**–CH_2OH	84.6±1.3	354.0±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
hexanol **nC_5H_{11}**–CH_2OH	84.4±1.3	353.1±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
benzyl alcohol **C_6H_5**–CH_2OH	98.8±1.3	413.4±5.4	Derived from Δ_fH^o in ref.	1986PED/NAY
2-propanol **CH_3**–$CH(CH_3)OH$	87.9±1.2	409.6±5.0	Derived from Δ_fH^o in ref.	1986PED/NAY

2-butanol **C_2H_5**–CH(CH_3)OH	86.0±1.2	359.8±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-pentanol **C_3H_7**–CH(CH_3)OH	86.1±1.2	360.2±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-methyl-2-butanol **iC_3H_7**–CH(CH_3)OH	83.9±1.3	351.0±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl alcohol **CH_3**–C(CH_3)$_2$OH	83.5±1.2	349.4±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-2-butanol **C_2H_5**–C(CH_3)$_2$OH	81.2±1.2	339.7±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-pentanol **C_2H_5**–CH(C_2H_5)OH	84.8±1.2	354.8±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethylene glycol **HOH_2C**–CH_2OH	85.6±1.5	358.2±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,2-propylene glycol **CH_3CH(OH)**–CH_2OH	86.2±1.8	360.7±7.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
1,2-propanediol **HOCH_2**–CH(CH_3)OH	84.2±1.3	352.3±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,3-butanediol **OH(CH_3)CH**–CH(CH_3)OH	90.5±1.5	378.7±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-aminoethan-1-ol **NH_2CH_2**–CH_2OH	80.2±2.5	335.6±10.5	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR

(continued)

Table 4.5.1 (continued) C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
ethyl methyl ether **CH_3**–CH_2OCH_3	86.8±1.2	363.2±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl propyl ether **C_2H_5**–CH_2OCH_3	85.3±1.2	356.9±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,2-methyloxyethane **CH_3OCH_2**–CH_2OCH_3	81.0±2.5	338.9±10.5	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
2-ethyl furan 	75± 2	313.8±8.4	VLPP	1981STE
6-(tert-butyl)-2-[3-(tert-butyl)-2-hydroxyphenyl]phenyl 	83.1	347.7	EPR	2001LUC/PED
acetaldehyde **CH_3**–C(O)H	84.8±0.4	354.8±1.7	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
trichloroacetaldehyde **CCl_3**–C(O)H	73.9±1.2	309.2±5.0	Derived from $\Delta_f H^o$ in ref.	2002CRC
acetyl fluoride **CH_3**–C(O)F	99.8±1.5	417.6±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC

acetyl chloride **CH_3**–C(O)Cl	87.9±1.5	367.8±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
trichloroacetyl chloride **CCl_3**–C(O)Cl	69.1±1.5	289.1±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
dichloroacetyl chloride **$CHCl_2$**–C(O)Cl	74.7±2	312.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
chloroacetyl chloride **$CClH_2$**–C(O)Cl	81.3±2	340.2±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
propanal **C_2H_5**–C(O)H	82.7±0.5	346.0±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-2-butenal **CH_3CH**=CH–C(O)H	97.8±2.0	409.2±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butanal **C_3H_7**–C(O)H	82.7±1.0	346.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpropanal **iC_3H_7**–C(O)H	82.5±1.2	345.2±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentanal **nC_4H_9**–C(O)H	83.2±0.7	348.1±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
heptanal **nC_6H_{13}**–C(O)H	81.0±2.0	338.9±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
benzaldehyde **C_6H_5**–C(O)H	97.6±1.0	408.4±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.5.1 (continued) C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
propanal **CH_3**–$CH_2C(O)H$	82.0±2.4	343.1±10.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butanal **C_2H_5**–$CH_2C(O)H$	79.8±2.5	333.9±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentanal **C_3H_7**–$CH_2C(O)H$	80.9±2.5	338.5±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
heptanal **C_5H_{11}**–$CH_2C(O)H$	78.5±3	328.4±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-phenylpropanone **$C_6H_5CH_2$**–$CH_2C(O)H$	67.9±1.5	284.1±6.3	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
dimethyl ketone **CH_3**–$C(O)CH_3$	84.1±0.5	351.9±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
bromoacetone **CH_2Br**–$C(O)CH_3$	85.9±1.5	359.4±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
chloroacetone **CH_2I**–$C(O)CH_3$	83.5±2.5	349.4±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl methyl ketone **CH_3**–$C(O)C_2H_5$	84.3±0.5	352.7±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl methyl ketone **C_2H_5**–$C(O)CH_3$	83.0±0.7	347.3±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

diethyl ketone $\mathbf{C_2H_5}$–C(O)C_2H_5	82.3±1.2	344.3±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl propyl ketone $\mathbf{C_3H_7}$–C(O)CH_3	83.3±0.7	348.5±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl propyl ketone $\mathbf{C_3H_7}$–C(O)C_2H_5	82.3±1.3	344.3±5.4	Derived from $\Delta_f H^o$ in ref.	1994PED
iso-propyl methyl ketone $\mathbf{iC_3H_7}$–C(O)CH_3	81.3±0.9	340.2±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iso-propyl ethyl ketone $\mathbf{iC_3H_7}$–C(O)C_2H_5	81.6±1.5	341.4±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
butyl methyl ketone $\mathbf{nC_4H_7}$–C(O)CH_3	82.9±1.3	346.9±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl methyl ketone $\mathbf{tC_4H_9}$–C(O)CH_3	78.7±1.0	329.3±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl ethyl ketone $\mathbf{tC_4H_9}$–C(O)C_2H_5	78.8±1.0	329.7±4.2	Derived from $\Delta_f H^o$ in ref.	1994PED
benzyl methyl ketone $\mathbf{C_6H_5CH_2}$–C(O)CH_3	70.1±2	293.3±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
benzyl phenyl ketone $\mathbf{C_6H_5CH_2}$–C(O)C_6H_5	71.2±3	297.9±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl methyl ketone $\mathbf{CH_3}$–CH_2C(O)CH_3	86.5±3	361.9±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.5.1 (continued) C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
butyl methyl ketone **C_3H_7**–$CH_2C(O)CH_3$	82.4±1.5	344.8±6.3	Derived from Δ_fH^o in ref.	2002CRC
trifluoromethyl phenyl ketone **CH_3**–$C(O)C_6H_5$	85.0	355.6	Photolysis	1997ZHA/CHE
trifluoromethyl phenyl ketone **CF_3**–$C(O)C_6H_5$	73.8±2	308.8±8.4	VLPP	1977COL/ZAB
ethyl phenyl ketone **C_2H_5**–$C(O)C_6H_5$	82.2±2.8	343.9±11.7	Derived from Δ_fH^o in ref.	1986PED/NAY
diphenyl ketone **C_6H_5**–$C(O)C_6H_5$	94.7±4	396.2±16.7	Derived from Δ_fH^o in ref.	1988LIA/BAR
benzyl phenyl ketone **$PhCH_2$**–C(O)Ph	71.2±3.5	297.9±14.6	Derived from Δ_fH^o in ref.	1986PED/NAY
bibenzyl ketone **$PhCH_2$**–$C(O)CH_2Ph$	65.4	273.6	Review	1982MCM/GOL
1,2-propanedione **$CH_3C(O)$**–C(O)H	72.3±2.0	302.5±8.4	Derived from Δ_fH^o in ref.	2002CRC
biacetyl **$CH_3C(O)$**–$C(O)CH_3$	73.4±1.0	307.1±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY

bibenzoyl **$C_6H_5C(O)$**–$C(O)C_6H_5$	68.9±4	288.3±16.7	Review	1982MCM/GOL
2,4-pentanedione **$CH_3C(O)$**–$CH_2C(O)CH_3$	80.8±2	338.1±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
acetic acid **CH_3**–C(O)OH	92.0±2	384.9±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
trifluoroacetic acid **CF_3**–C(O)OH	88.6±2	370.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
chloroacetic acid **$CClH_2$**–C(O)OH	85.5±2	357.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
bromoacetic acid **CH_2Br**–C(O)OH	85.6±2	358.2±8.4	Derived from $\Delta_f H^o$ in ref.	2001DOR/NOV
glycine **NH_2CH_2**–C(O)OH	83.5±2	349.4±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
N-methylglycine **CH_3NHCH_2**–C(O)OH	71.8±2	300.4±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
propenoic acid **C_2H_3**–C(O)OH	104.1±2	435.5±8.4	Derived from $\Delta_f H^o$ in ref.	1998NIST
propanoic acid **C_2H_5**–C(O)OH	90.8±1.5	379.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-chloropropanoinc acid **CH_3CHCl**–C(O)OH	85.5±2	357.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC

(continued)

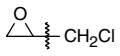
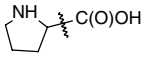
Table 4.5.1 (continued) C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
butanoic acid **C_3H_7**–C(O)OH	91.0±1.5	380.7±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentanoic acid **C_4H_9**–C(O)OH	89.7±1.5	375.3±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
3-methylbutanoic acid **sC_4H_9**–C(O)OH	91.6±3	383.3±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethylpropanoic acid **tC_4H_9**–C(O)OH	82.5±4	345.2±16.7	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
hexanoic acid **C_5H_{11}**–C(O)OH	88.8±1.5	371.5±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
heptanoic acid **C_6H_{13}**–C(O)OH	89.7±1.5	375.3±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
benzoic acid **Ph**–C(O)OH	102.7±2	429.7±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
2-phenylacetic acid **$PhCH_2$**–C(O)OH	67	280.3	Review	1970ONE/BEN
diphenylacetic acid **Ph_2CH**–C(O)OH	59.4±3	248.5±12.6	Review	1970ONE/BEN
naphthlene-1-carboxylic acid **$C_{10}H_7$**-1-C(O)OH	102.8±2.0	430.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

naphthlene-2-carboxylic acid **$C_{10}H_7$**-2-C(O)OH	104.8±2.0	438.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
glycolic acid **$HOCH_2$**–C(O)OH	88.8±1.3	371.5±5.4	Derived from $\Delta_f H^o$ in ref.	2001DOR/NOV
oxalic acid **HOC(O)**–C(O)OH	80.0±1.5	334.7±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
sarcosine **CH_3NHCH_2**–C(O)OH	72.0±4	301.2±16.7	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
L-alanine **$CH_3CH(NH_2)$**–C(O)OH	79.2±4	331.4±16.7	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
acetic acid methyl ester **CH_3**–C(O)OCH_3	86.2±3	360.7±12.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl acrylate **C_2H_3**–C(O)OCH_3	110.7±1.5	463.2±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
butanoic acid **C_2H_5**–CH_2C(O)OH	81.9±3	342.7±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
β-alanine **NH_2CH_2**–CH_2C(O)OH	77.1±4	322.6±16.7	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
dimethyl oxalate **$CH_3OC(O)$**–C(O)OCH_3	76.3±1.5	319.2±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
diketene **O=C=CH**–CH=C=O	129.3±2.5	541.0±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC

(continued)

Table 4.5.1 (continued) C–C BDEs in Organic Compounds Containing Oxygen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-chlorooxirane 	89.8±2.5	375.7±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyoxirane 	93.5±2.5	391.2±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
proline 	74.6±2.5	312.1±10.5	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR

4.5.2 *Organic compounds containing nitrogen atoms*

Table 4.5.2 C–C BDEs in Organic Compounds Containing Nitrogen Atoms

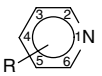
The broken bonds (**boldface =** dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyanogen **CN**–CN	(1) 137.7±1.6	576.1±6.7	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 137.1	573.6	(2) Derived	(2) 2002MAT/LEB
formyl cyanide HC(O)–**CN**	109.3±2	457.3±8.4	Derived from $\Delta_f H^o$ in ref.	1996BOR/ING
thioformyl cyanide HC(S)–**CN**	127.2±2	532.2±8.4	Derived from $\Delta_f H^o$ in ref.	1996BOR/ING
trifluoroacetonitrile CF_3–**CN**	134.1±2	561.0±8.4	Derived	1982MCM/GOL

acetonitrile CH_3–**CN**	(1) 125.2±2.2 (2) 124.7	523.8±9.2 521.7	(1) Derived from $\Delta_f H^o$ in ref. (2) Derived	(1) 1986PED/NAY (2) 2002MAT/LEB
ethynylnitrile CH≡C–**CN**	143.9	602.1	Photolysis	1973OKA/DIB
2-propenenitrile CH_2CH–**CN**	133.9±1.8	560.2±7.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propanenitrile C_2H_5–**CN**	121.6±1.8	508.7±7.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-butenenitrile $CH_2CH=CH_2$–**CN**	111.4±2	466.1±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
butanenitrile C_3H_7–**CN**	121.3±2.0	507.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpropanenitrile iC_3H_7–**CN**	120.9±2.0	505.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentanenitrile nC_4H_9–**CN**	121.6±2.0	508.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethylpropanenitrile tC_4H_9–**CN**	117.7±2.0	492.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclobutanecarbonitrile c-C_4H_7–**CN**	122.7±2.0	513.4±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclopentanecarbonitrile c-C_5H_9–**CN**	120.5±2.0	504.2±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.5.2 (continued) C–C BDEs in Organic Compounds Containing Nitrogen Atoms

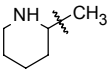
The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyclohexanecarbonitrile c-C_6H_{11}–**CN**	122.4±2.0	512.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
benzonitrile C_6H_5–**CN**	132.8±2.0	555.6±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
heptanenitrile nC_6H_{13}–**CN**	120.9±2.0	505.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propanenitrile **CH_3**–CH_2CN	83.2±3	348.1±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butanenitrile **C_2H_5**–CH_2CN	(1) 76.9±1.7 (2) **80.8±2**	321.7±7.1 **338.1±8.4**	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1975KIN/GOD (2) 1986PED/NAY
3-butenenitrile **C_2H_3**–CH_2CN	110.4±2	461.9±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
pentanenitrile **nC_3H_7**–CH_2CN	81.7±3	341.8±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylbutanenitrile **iC_3H_7**–CH_2CN	73±2	305.4±8.4	VLPP	1975KIN/GOD
heptanenitrile **nC_5H_{11}**–CH_2CN	80.8±3	338.1±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

octanenitrile **nC_6H_{13}**–CH_2CN	80.5±3	336.8±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methylpropanenitrile **CH_3**–$CH(CH_3)CN$	(1) 78.8±2 (2) **79.5±2**	329.7±8.4 **332.6±8.4**	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1975KIN/GOD (2) 1986PED/NAY
2,2-dimethyl propanenitrile **CH_3**–$C(CH_3)_2CN$	(1) 74.7±1.6 (2) 81.4±4	312.5±6.7 340.6±16.7	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1976KIN/GOD (2) 1998NIST
propanedinitrile $(CN)CH_2$–**CN**	102.4±3	428.4±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butanedinitrile $(CN)CH_2$–**CH_2CN**	70.7±4	295.8±16.7	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tetramethylbutanedinitrile $(CN)C(CH_3)_2$–**$C(CH_3)_2$CN**	61.2±3	256.1±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methy-2-phenyl-propanenitrile **CH_3**–$C(CH_3)(CN)C_6H_5$	59.9	250.6	Pyrolysis	1982MEO
pyridine, substituted **R**-pyridyl 				
R = 2-Me	(1) 97.9±2	409.6±8.4	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
3-Me	(1) 103.2±2	431.8±8.4		
4-Me	(1) 103.7±2	433.9±8.4		
2-CH_2Ph	(2) 86.7	362.8	(2) VLPP	(2) 1984ROS/MCM

(continued)

Table 4.5.2 (continued) C–C BDEs in Organic Compounds Containing Nitrogen Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-methyl-piperidine **CH_3**-pyrerid-2-yl	83.4±2	348.9±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-piperidine **CH_3**-pyrerid-2-yl	83.4±2	348.9±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-ethylpyridine **CH_3**-2-pyridylmethyl	75.5±2.9	315.9±12.1	VLPP	1981BAR/STE
3-ethylpyridine **CH_3**-3-pyridylmethyl	73.9±2.6	309.2±10.9	VLPP	1981BAR/STE
4-ethylpyridine **CH_3**-4-pyridylmethyl	74.6±2.6	312.1±10.9	VLPP	1981BAR/STE
ethylamine **CH_3**–CH_2NH_2	82.7±2.3	346.0±9.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propylamine **C_2H_5**–CH_2NH_2	81.5±2.3	341.0±9.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
phenylmethylamine **C_6H_5**–CH_2NH_2	94.2±2.5	394.1±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
benzyl methylamine **$C_6H_5CH_2$**–CH_2NH_2	68.0±2	284.5±8.4.0	Pyrolysis	1977COL/BEN
2-propylamine **CH_3**–$CH(CH_3)NH_2$	81.8±2.3	342.3±9.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

2-methylpropylamine **CH$_3$**–C(CH$_3$)$_2$NH$_2$	73.4±2.5	307.1±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,2-ethanediamine **NH$_2$CH$_2$**–CH$_2$NH$_2$	68.4±3	286.2±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,2-propanediamine **NH$_2$CH$_2$**–CH(CH$_3$)NH$_2$	75.8±3	317.1±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-1,2-propanediamine **NH$_2$CH$_2$**–C(CH$_3$)$_2$NH$_2$	74.6±3	312.1±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-(2-pyridyl)pyridine **NC$_5$H$_4$**–C$_5$H$_4$N	103.9±3	434.7±12.6	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
2-methylpiperidine 	83.9±3	351.0±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

4.5.3 *Organic compounds containing sulfur atoms*

Table 4.5.3 C–C BDEs in Organic Compounds Containing Sulfur Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
ethylthiol **CH$_3$**–CH$_2$SH	82.5±2.2	345.2±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-propanethiol **C$_2$H$_5$**–CH$_2$SH	80.9±2.4	338.5±10.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-butanethiol **C$_3$H$_7$**–CH$_2$SH	81.1±2.5	339.3±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 4.5.3 (continued) C–C BDEs in Organic Compounds Containing Sulfur Atoms

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-methyl-1-propanethiol **iC_3H_7**–CH_2SH	80.6±2.5	337.2±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
1-pentanethiol **C_4H_9**–CH_2SH	81.2±2.5	339.7±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
2-methyl-1-butanethiol **sC_4H_9**–CH_2SH	80.0±2.5	334.7±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
3-methyl-1-butanethiol **iC_4H_9**–CH_2SH	80.5±2.5	336.8±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
2,2-dimethyl-1-propanethiol **tC_4H_9**–CH_2SH	78.7±2.5	329.3±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
1-hexanethiol **nC_5H_{11}**–CH_2SH	80.3±2.5	336.0±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
1-heptanethiol **nC_6H_{13}**–CH_2SH	80.2±2.5	335.6±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
phenylmethane-1-thiol **C_6H_5**–CH_2SH	93.2±2.5	389.9±10.5	Derived from Δ_fH^o in ref.	1986PED/NAY
1,2-ethanethiol **$HSCH_2$**–CH_2SH	74.9±2.8	313.4±11.7	Derived from Δ_fH^o in ref.	1986PED/NAY
ethyl methyl sulfide **CH_3**–CH_2SCH_3	82.0±2.0	343.1±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY

methyl propyl sulfide $\mathbf{C_2H_5}$–CH_2SCH_3	80.8±2.0	338.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl phenyl sulfide $\mathbf{CH_3}$–$CH_2SC_6H_5$	80.9±2.0	338.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dibenzyl sulfide $\mathbf{C_6H_5}$–$CH_2SC_6H_5$	97.1±2.0	406.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

chapter five

Tabulated BDEs of C–halogen bonds

5.1 C–F bonds

Table 5.1 C–F BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
cyanogen fluoride **F**–CN	112.3±1.2	469.9±5.0	AE	1978DAY/GOW
tetrafluoromethane **F**–CF_3	129.6±1.0	542.2±4.2	Recommend.	1998CHA
trifluoromethane **F**–CHF_2	(1) 127 (2) **127.6±1.4**	531.4 **533.9±5.9**	(1) Bromination (2) Review	(1) 1987TSC/PAD (2) 2001LAZ/PRO
difluoromethane **F**–CH_2F	118.6±2.1	496.2±8.8	Review	2001LAZ/PRO
chlorofluoromethane **F**–CF_2Cl	117±6	489.5±25.1	Kinetics	1972FOO/TAI(b)
dichlorofluoromethane **F**–$CFCl_2$	110± 6	460.2±25.1	Kinetics	1972FOO/TAI(b)

(continued)

Table 5.1 (continued) C–F BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
chlorodifluoromethane **F**–CHFCl	110.5±2.4	462.3±10.0	Derived	1987TSC/PAD
chlorofluoromethane **F**–CH_2Cl	111.2±2.3	465.3±9.6	Derived	1987TSC/PAD
fluoroiodomethane **F**–CH_2I	≤110.0	≤460.2	Infrared chemiluminescence	2002ARU/VIJ
fluoromethane **F**–CH_3	(1) 112.8 (2) **110.0±2.0** (3) 109.8±1.2	472.0 **460.2±8.4** 459.4±5.0	(1) Review (2) Derived from $\Delta_f H^o$ in ref. (3) Review	(1) 1988LIA/BAR (2) 1998CHA (3) 2001LAZ/PRO
difluoroethyne **F**–C≡CF	124±5	518.8±21	Review	1996ZAR/WES
tetrafluoroethylene **F**–CF=CF_2	130.6±3	546.4±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
hexafluoroethane **F**–CF_2CF_3	(1) 126.8±1.8 (2) **127.2±1.5**	530.5±7.5 **532.2±6.3**	(1) Derived (2) Review	(1) 1982MCM/GOL (2) 2001LAZ/PRO
1,1,1,2-tetrafluoroethane **F**–CH_2CF_3	109.4	457.7	Derived	1975CHE/ROD
1,1,1-trifluoroethane **F**–CF_2CH_3	124.8±2	522.2±8.4	Derived	1975CHE/ROD

vinyl fluoride **F**–C_2H_3	123.7±3	517.6±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
fluoroethane **F**–C_2H_5	113.1±2	473.1±8.4	Derived from $\Delta_f H^o$ in ref.	1998SMI
1-fluopropane **F**–C_3H_7	(1) 111.1±3 (2) **113.5±2**	464.8±12.6 **474.9±8.4**	(1) Derived from $\Delta_f H^o$ in ref. (2) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY (2) 1998SMI
2-fluopropane **F**–iC_3H_7	(1) 110.1±5 (2) **115.4±2**	460.7±20.9 **482.8±8.4**	(1) Derived from $\Delta_f H^o$ in ref. (2) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY (2) 1998SMI
2-fluoro-2-methylpropane **F**–tC_4H_9	117.0±2	489.5±8.4	Derived from $\Delta_f H^o$ in ref.	1998SMI
fluorobenzene **F**–C_6H_5	125.6±2	525.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
hexafluorobenzene **F**–C_6F_5	114	477.0	Derived	1975CHO/GOL
fluorocyclohexane **F**–c-C_6H_{11}	117.4±2	491.2±8.4	Derived from $\Delta_f H^o$ in ref.	1997SCH/VER
(fluoromethyl)benzene **F**–$CH_2C_6H_5$	97.6±2	408.4±8.4	Derived from $\Delta_f H^o$ in ref.	(1) 1997SCH/VER (2) 2002VER/KRA
formyl fluoride **F**–COH	119.0±2.5	497.9±10.5	Derived from $\Delta_f H^o$ in ref.	1998CHA

(continued)

Table 5.1 (continued) C–F BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
fluoroformyl fluoride **F**–COF	127.9±3	535.1±12.6	PIMS	1995BUC/JOH
acetyl fluoride **F**–C(O)CH_3	122.3±3	511.7±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC

5.2 C–CI bonds

Table 5.2 C–CI BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyanogen chloride **Cl**–CN	(1) 100.8±1.2 (2) **101.5±2.0**	421.7±5.0 **424.7±8.4**	(1) AP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1978DAY/GOW (2) 2002CRC
trichlorofluoromethane **Cl**–$CFCl_2$	(1) **72±2** (2) 70.5	**301.2±8.4** 295.0	(1) Kinetics (2) Electron capture detection	(1) 1972FOO/TAI(b) (2) 1989CHE/ALB
dichlorodifluoromethane **Cl**–CF_2Cl	(1) 76±2 (2) 73.4±2.5 (3) **76.4±2.0**	318.0±8.4 307.1±10.5 **319.7±8.4**	(1) Kinetics (2) Electron capture detection (3) Derived from $\Delta_f H^o$ in ref.	(1) 1972FOO/TAI(b) (2) 1989CHE/ALB (3) 2002CRC
chlorotrifluoromethane **Cl**–CF_3	(1) 86.1±0.8 (2) 86.2±3	360.2±3.3 360.7±12.6	(1) Kinetics (2) Kinetics	(1) 1967COO/WHI (2) 1983MAR/PAR

	(3) **85.8±1.3**	**359.0±5.4**	(3) Review	(3) 1998CHA
	(4) 89.1	372.8	(4) Electron capture detection	(4) 1989CHE/ALB
chlorofluoromethane **Cl**–CH_2F	84.7±2.8	354.4±11.7	Derived	1987TSC/PAD
dichlorofluoromethane **Cl**–CHFCl	(1) **82.7±3.2**	**346.0±13.4**	(1) Derived	(1) 1987TSC/PAD
	(2) 83.4	348.9	(2) Electron capture detection	(2) 1989CHE/ALB
tetrachloromethane **Cl**–CCl_3	(1) 70.4±1	294.6±4.2	(1) Bromination	(1) 1973MEN/GOL
	(2) 70.8±1.3	296.2±5.4	(2) Correlation	(2) 1978KAT/RAJ
	(3) 70	292.9	(3) Derived	(3) 1983WEI/BEN
	(4) **70.9**	**296.6**	(4) Review	(4) 2001LAZ/PRO
trichloromethane **Cl**–$CHCl_2$	(1) 76.2	318.8	(1) Correlation	(1) 1978KAT/RAJ
	(2) 80.9±1	338.5±4.2	(2) Derived	(2) 1987TSC/PAD
	(3) 73.6	307.9	(3) Electron capture detection	(3) 1989CHE/ALB
	(4) **76.6±1.5**	**320.5±6.3**	(4) Review	(4) 2001LAZ/PRO
dichloromethane **Cl**–CH_2Cl	(1) 79.3	331.8	(1) Correlation	(1) 1978KAT/RAJ
	(2) 80.9±1.0	338.5	(2) Derived	(2) 1987TSC/PAD
	(3) 77.9	325.9	(3) Electron capture detection	(3) 1989CHE/ALB
	(4) **80.8**	**338.1**	(4) Review	(4) 2001LAZ/PRO
	(5) 78.5	328.4	(5) Correlation	(5) 1995DEN
chloroiodomethane **Cl**–CH_2I	≤ 72.0	≤ 301.2	Infrared chemiluminescence	2002ARU/VIJ
chloromethane **Cl**–CH_3	83.7±0.4	350.2±1.7	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 5.2 (continued) C–CI BDEs

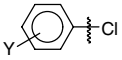
The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
chloroethyne **Cl**–C≡CH	104.1±2	435.6±8.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
2-chloroethanenitrile **Cl**–CH_2CN	63.9	267.4	CID	2002POU/UPS
(Z)-1,2-dichloroethylene (Z)-ClCH=CH–**Cl**	88.2	369.0	Electron capture detection	1989CHE/ALB
(E)-1,2-dichloroethylene (E)-ClCH=CH–**Cl**	88.4	369.9	Electron capture detection	1989CHE/ALB
1,2-dichloroethylene g-CH2=CCl–**Cl**	93.4	390.8	Electron capture detection	1989CHE/ALB
1,1,2-trichloroethylene ClCH=CCl–**Cl**	93.6	391.6	Electron capture detection	1989CHE/ALB
tetrachloroethylene CCl_2=CCl–**Cl**	91.7	383.7	Electron capture detection	1989CHE/ALB
vinyl chloride **Cl**–CH=CH_2	91.7±1.0	383.7±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
chlorotrifluoroethylene **Cl**–CF=CF_2	103.9±2	434.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC

chloropentafluoroethane **Cl**–CF_2CF_3	**(1) 82.7±1.7** (2) 78±2 (3) 82.0±1.2	**346.0±7.1** 326.4±8.4 343.1±5.0	Kinetics	(1) 1967COO/WHI (2) 1972FOO/TAI(b) (3) 1989TAC/SAL
dichlorotetrafluoroethane **Cl**–CF_2CF_2Cl	(1) 78±2 (2) 79.2±5	326.4±8.4 331.4±20.9	Kinetics	(1) 1972FOO/TAI(b) (2) 1989TAC/SAL
1,1,1-trichloro-2, 2,2-trifluoroethane **Cl**–CCl_2CF_3	(1) 71 (2) 73.6	297.1 307.9	Correlation	(1) 1978KAT/RAJ (2) 1995DEN
hexachloroethane **Cl**–CCl_2CCl_3	(1) **72.6** (2) 71.7 (3) 71.5	**303.8** 300.0 299.2	(1) Photochlorin. (2) Correlation (3) Derived	(1) 1969FRA/HUY (2) 1995DEN (3) 1997CIO/LIU
pentachloroethane **Cl**–$CHClCCl_3$	79.0±1	330.5±4.2	Pyrolysis	1982BEN/WEI
pentachloroethane **Cl**–CCl_2CHCl_2	(1) 67.8 (2) 74.5	283.7 311.7	(1) Derived (2) Correlation	(1) 1997CIO/LIU (2) 1995DEN
1,1,1,2-tetrachloroethane **Cl**–CCl_2CH_2Cl	76.0	318.0	Correlation	1995DEN
1,1,1-trichloroethane **Cl**–CCl_2CH_3	(1) 70 (2) 78.5	292.9 328.4	Correlation	(1) 1978KAT/RAJ (2) 1995DEN
1,1-dichloroethane **Cl**–$CHClCH_3$	(1) 79.5±2.1 (2) **78.4±0.4**	332.6±8.8 **327.9±1.8**	Derived	(1) 1997CIO/LIU (2) 1998SE
1,2-dichloroethane **Cl**–CH_2CH_2Cl	(1) 79.1 (2) 83.2±2.3 (3) **82.5±1.2**	331.0 348.1±9.6 **345.1±5.0**	(1) Electron capture detection (2) Derived (3) Derived	(1) 1989CHE/ALB (2) 1997CIO/LIU (3) 1998SEE

(continued)

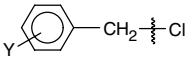
Table 5.2 (continued) C–CI BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1,1-bromochloroethane **Cl**–$CHBrCH_3$	79.3±2.0	331.8±8.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
chloroethane **Cl**–CH_2CH_3	84.2±0.8	352.3±3.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-chloro-1-propene **Cl**–$CH_2CH{=}CH_2$	71.3±1.2	298.3±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-chloro-2-methyl-1-propene **Cl**–$CH_2C(CH_3){=}CH_2$	66.2	277.0	Correlation	1995DEN
1-chloropropane **Cl**–nC_3H_7	84.3±1.0	352.7±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,3-dichloropropane **Cl**–$CH_2CH_2CH_2Cl$	83.4	348.9	Electron capture detection	1989CHE/ALB
2-chloropropane **Cl**–iC_3H_7	84.6±1.5	354.0±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,4-dichloro-2-butene **Cl**–$CH_2CH{=}CHCH_2Cl$	67.0	280.3±6.3	Correlation	1995DEN
1-chlorobutane **Cl**–nC_4H_9	84.5±1.0	353.5±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-chloro-2-methylpropane **Cl**–iC_4H_9	83.8±1.5	350.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

2-chlorobutane **Cl**–sC_4H_9	83.7±1.5	350.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-chloro-2-methylpropane **Cl**–tC_4H_9	84.1±1.5	351.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-chloropentane **Cl**–nC_5H_{11}	83.8±1.5	350.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-chloro-2-methylbutane **Cl**–$C(CH_3)_2(C_2H_5)$	84.3±1.5	352.7±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-chlorohexane **Cl**–$CH(CH_3)(C_4H_9)$	84.8±1.5	354.8±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
chlorocyclohexane **Cl**–cycloC_6H_{11}	86.1±2	360.2±6.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
chlorobenzene, substituted  				
Y = H	(1) 95.5±1.5 (2) 95.1±2.5	399.6±6.3 397.9±10.5	(1) Derived from $\Delta_f H^o$ in ref. (2) Electron capture detection	(1) 1986PED/NAY (2) 1989CHE/ALB
2-Cl	(2) 92.2	385.8		
3-Cl	(2) 89.9	376.1		
4-Cl	(2) 93.7	392.0		
2-Me	(2) 93.7	392.0		
2-CF_3	(2) 93.0	389.1		
4-CF_3	(2) 93.0	389.1		
3-CH_3CO	(2) 92.2	385.8		
4-CH_3CO	(2) 91.4	382.4		

(continued)

Table 5.2 (continued) C–Cl BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
3-F-4-Cl	(2) 91.6	383.3		
2-CF_3-4-Cl	(2) 90.3	377.8		
3,5-Cl_2	(2) 94.5	395.4		
2,4,5-Cl_3	(2) 94.4	395.0		
chloropentafluorobenzene **Cl**–C_6F_5	91.6±2	383.3±8.4	Derived	1982MCM/GOL
chlorocyclohexane **Cl**–C_6H_{11}	85.1±2	356.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
trichloro phenyl methane **Cl**–$CCl_2C_6H_5$	66.5	278.2	Correlation	1995DEN
benzyl chloride **Cl**–$CH_2C_6H_5$	(1) **72.9±2**	**305.0±8.4**	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 71.6	299.6	(2) Electrochem.	(2) 1992AND/GOR
benzyl chloride, substituted 				
Y = 3-F	68.5	286.8	Correlation	1998DEN
4-F	69.1	289.0		
3-Cl	69.1	289.0		
3-Me	69.1	289.0		
4-Me	69.9	292.5		
3-CF_3	68.4	286.2		
3-MeO	69.2	289.6		

4-tBu	69.8	291.9		
4-CN	67.0	280.3		
3,4-Cl_2	68.3	285.6		
3,5-Cl_2	66.7	279.2		
3,5-$(CF_3)_2$	66.3	277.6		
1-chloronaphthalene **Cl**-1-naphthyl	(1) 93.4±3 (2) **96.3±2.7**	390.8±12.6 **402.9±11.3**	(1) Electron capture detection (2) Derived from $\Delta_f H^o$ in ref.	(1) 1989CHE/ALB (2) 1986PED/NAY
2-chloronaphthalene **Cl**–2-naphthyl	91.9±2.7	384.5±11.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-adamantyl chloride **Cl**–1-adamantyl	(1) 83.8±3 (2) 90.4±3	350.6±12.6 378.2±12.6	Derived from $\Delta_f H^o$ in ref.	(1) 1999FLO/DAV (2) 2002LI/BAE
2,2,2-trichloroethanenitrile $CNCCl_2$–**Cl**	62.2	260.2	Correlation	1995DEN
2,2-dichloroethanenitrile CNCHCl–**Cl**	70.7	295.8	Correlation	1995DEN
carbonyl chloride **Cl**–C(O)Cl	76.2±2	318.8±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
acetyl chloride **Cl**–$C(O)CH_3$	84.6±2	354.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chloroacetyl chloride **Cl**–$CH_2C(O)Cl$	64.7	270.7	Correlation	1995DEN

(continued)

Table 5.2 (continued) C–CI BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
benzoyl chloride **Cl**–C(O)C_6H_5	81.5±2	341.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chloro-1-phenylethan-1-one **Cl**–$CH_2C(O)C_6H_5$	73.9	309.0	VLPP	1999DOR/HEM
2-chloroacetic acid **Cl**–$CH_2C(O)OH$	(1) 66.6 (2) **74.3±0.5**	278.7 **310.9±2.2**	(1) Correlation (2) Calorimetry	(1) 1995DEN (2) 2001LAG/DIO
2,2-dichloroacetic acid **Cl**–CClHC(O)OH	67.2	281.2	Correlation	1995DEN
2,2,2-trichloroacetic acid **Cl**–$CCl_2C(O)OH$	66.3	277.4	Correlation	1995DEN
methyl 2-chloroacetate **Cl**–$CH_2C(O)OCH_3$	72.1	301.7	Correlation	1995DEN
ethyl 2,2-dichloroacetate **Cl**–CClHC(O)OC_2H_5	68.8	287.9	Correlation	1995DEN
ethyl 2,2,2-trichloroacetate **Cl**–$CCl_2C(O)OC_2H_5$	66.7	279.1	Correlation	1995DEN
phenyl 2-chloroacetate **Cl**–C(O)OC_6H_5	(1) 81 (2) **87**	338.9 **364.0**	(1) PAC (2) PAC, revised	(1) 1989SIM/GRI (2) 1999LAA/MUL

diethyl 2, 2-dichloropropane-1,3-dioate **Cl**–CCl(C(O)OEt)$_2$	67.3	281.6	Correlation	1995DEN
chlorothioformyl chloride **Cl**–C(S)Cl	63.4±0.5	265.3±2.1	Photolysis	1977OKA

5.3 C–Br bonds

Table 5.3 C–Br BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyanogen bromide **Br**–CN	87.8±1.2	367.4±5.0	AE	1978DAY/GOW
bromotrifluoromethane **Br**–CF_3	(1) 70.6±3.0	295.4±12.6	(1) Kinetics	(1) 1972FER/WHI(b)
	(2) 69.6	291.6	(2) Derived	(2) 1983EVA/WEE
	(3) 71.0	297.1	(3) Correlation	(3) 1995DEN
	(4) **70.8±0.3**	**296.2±1.3**	(4) PIMS	(4) 1997ASH/RUS
	(5) 69.4±1.2	290.4±5.0	(5) Review	(5) 1998CHA
bromotrichloromethane **Br**–CCl_3	55.3±1	231.4±4.2	Bromination	1973MEN/GOL
tetrabromomethane **Br**–CBr_3	56.2±1.8	235.1±7.5	Bromination	1971KIN/GOL
bromochlorodifluoromethane **Br**–CF_2Cl	64.5±1.5	269.9±6.3	Review	1982MCM/GOL
bromodifluoromethane **Br**–CHF_2	69±2	288.7±8.4	Bromination	1974OKA/WHI

(continued)

Table 5.3 (continued) C–Br BDEs

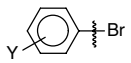
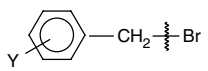
The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
tetrabromomethane **Br**–CBr_3	(1) 56.2±1.8 (2) **54.7±2.3**	235.1±7.5 **228.9±9.6**	(1) Bromination (2) Review	(1) 1971KIN/GOL (2) 2001LAZ/PRO
tribromomethane **Br**–$CHBr_2$	(1) 64.8 (2) **65.7±3.1**	271.1 **274.9±13.0**	(1) Electron capture detection (2) Review	(1) 1989CHE/ALB (2) 2001LAZ/PRO
dibromomethane **Br**–CH_2Br	(1) 69.8±2 (2) 65.8 (3) 69.3±2.4	292.0±8.4 275.3 **290.0±10.0**	(1) Bromination (2) Electron capture detection (3) Review	(1) 1987TSC/PAD (2) 1989CHE/ALB (2) 2001LAZ/PRO
bromomethane **Br**–CH_3	70.3±0.5	294.1±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-1,2-dibromoethylene (Z)-CHBr=CH–**Br**	<83.8	<350.6	Electron capture detection	1989CHE/ALB
(E)-1,2-dibromoethylene (E)-CHBr=CH–**Br**	<83.3	<348.5	Electron capture detection	1989CHE/ALB
vinyl bromide **Br**–$CH=CH_2$	79.4±1.5	332.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
bromopentafluoroethane **Br**–CF_2CF_3	(1) 68.6±1.5 (2) 68.8 (3) **67.7±1.5**	287.0±6.3 287.9 **283.3±6.3**	(1) Kinetics (2) Derived (3) Derived from $\Delta_f H^o$ in ref.	(1) 1972FER/WHI (2) 1983EVA/WEE (3) 2002CRC

1,1-dibromo-1-chloro-2,2,2-trifluoroethane **Br**–CClBrCF$_3$	60.0±1.5	251.0±6.3	Review	1982MCM/GOL
1-bromo-1-chloro-2,2,2-trifluoroethane **Br**–CHClCF$_3$	65.7±1.5	274.9±6.3	Review	1982MCM/GOL
1-bromo-1,1-difluoroethane **Br**–CF$_2$CH$_3$	68.6±1.3	287.0±5.4	Kinetics	1977PIC/ROD
1-bromo-2-chloroethane **Br**–CH$_2$CH$_2$Cl	69.9±2.0	292.5±8.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
1,1-bromochloroethane **Br**–CHClCH$_3$	65±2	272.0±8.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
bromoethane **Br**–C$_2$H$_5$	70.0±1.0	292.9±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-bromo-1-propene **Br**–CH$_2$CH=CH$_2$	56.7±1.2	237.2±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(E)-1-bromo-1-propene (E)-**Br**–CH=CHCH$_3$	80.0±1.2	334.7±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
(Z)-1-bromo-1-propene (Z)-**Br**–CH=CHCH$_3$	80.7±1.2	337.6±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-bromopropane **Br**–nC$_3$H$_7$	(1) 66.7 (2) **71.3±1.0**	279.1 **298.3±4.2**	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1983EVA/WEE (2) 1986PED/NAY

(continued)

Table 5.3 (continued) C–Br BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-bromopropane **Br**–iC_3H_7	(1) 65.5 (2) **71.5±1.5**	274.1 **299.2±6.3**	(1) Derived (2) Derived from $\Delta_f H^o$ in ref.	(1) 1983EVA/WEE (2) 2002CRC
1,3-dibromopropane **Br**–$CH_2CH_2CH_2Br$	77.6	324.7	Electron capture detection	1989CHE/ALB
1-bromo-heptafluoropropane **Br**–$CF_2CF_2CF_3$	66.5±2.5	278.2±10.5	Kinetics	1967COO/WHI
2-bromo-heptafluoropropane CF_3CF**Br**CF_3	(1) 65.5±1.1 (2) 65.4	274.1±4.6 273.6	(1) Review (2) Kinetics	(1) 1982MCM/GOL (2) 1983EVA/WEE
1,1,1-tribromopropane **Br**–$CBr_2CH_2CH_3$	60.8	254.4	Correlation	1995DEN
1-bromobutane **Br**–nC_4H_9	70.9±1	296.6±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-bromobutane **Br**–sC_4H_9	71.7±1	300.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-bromo-2-methylpropane **Br**–tC_4H_9	70.0±1.5	292.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-bromopentane **Br**–nC_5H_{11}	70.5±1	295.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

1-bromohexane **Br**–nC_6H_{13}	70.1±1	293.3±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
bromobenzene, substituted				
 Y = H	(1) 83.5±2.5	349.4±10.5	(1) Electron capture detection	(1) 1989CHE/ALB
	(2) **80.4±1.5**	**336.4±6.3**	(2) Derived from $\Delta_f H^o$ in ref.	(2) 1986PED/NAY
2-F	(3) 82.0	343.1	(3) Correlation	(3) 1995DEN
2-Me	(3) 83.9	351.0		
3-CF3	(3) 79.9	334.3		
bromotoluene, substituted				
 Y = p-H	(1) 60.0±3	251.1±12.6	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 55.9	233.9	(2) Electrochem.	(2) 1992AND/GOR
	(3) 60.7±1	254±4	(3) PAC	(3) 1997LAA/BOR
	(4) 55.1±2.5	230.5±10.5	(4) Derived from $\Delta_f H^o$ in ref.	(4) 1998NIST
	(5) **56.1±2**	**234.7±8.4**	(5) Derived from $\Delta_f H^o$ in ref.	(5) 2002VER/KRA
p-F	(6) 58.9	246.4	(6) AOP	(6) 1993ZHA
p-Br	(6) 57.6	241.0		
p-CN	(1) 60.9±1 (6) **54.4**	255±4 **227.6**		
p-Me	(6) 59.7	249.8		
p-t-Bu	(1) 60.0±1	251±4		
m-CF_3	(1) 60.9±1	255.0±4		
(1-bromovinyl)benzene CH_2=CH**Br**Ph	63.4	265.3	Correlation	1995DEN
(2-bromovinyl)benzene **Br**–CH=CHPh	65.1	272.4	Correlation	1995DEN

(continued)

Table 5.3 (continued) C–Br BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
benzyl bromide **Br**–$CH_2C_6F_5$	53.8±1.5	225.1±6.3	Toluene carrier tech	1980KOM/KRE
(1,2,2,2-tetraethyl)benzene **Br**–$CBr_2CHBrPh$	60.3	252.3	Correlation	1995DEN
1-bromonaphthalene **Br**–$C_{10}H_7$	79.3	331.8	Electron capture detection	1989CHE/ALB
(1,2-dibromo-2-phenylethyl)-benzene $(PhCH\mathbf{Br})_2$	62.9	263.2	Correlation	1995DEN
acetyl bromide **Br**–$C(O)CH_3$	(1) 64 (2) 69.8±2	267.8 292.0±8.4	(1) Photolysis (2) Derived from $\Delta_f H^o$ in ref.	(1) 1995SU/DIB (2) 2002CRC
benzoyl bromide **Br**–$C(O)C_6H_5$	(1) 64.1 (2) **66.1±2**	268.2 **276.6±8.4**	(1) Review (2) Derived from $\Delta_f H^o$ in ref.	(1) 1970ONE/BEN (2) 1994PED
1-bromoacetone **Br**–$CH_2C(O)CH_3$	62.5	261.5	VLPP	1978ZAB/BEN
2-bromo-1-phenylethan-1-one **Br**–$CH_2C(O)C_6H_5$	64.8	271.0	VLPP	1999DOR/HEM
2-bromoacetic acid **Br**–$CH_2C(O)OH$	(1) 63.6 (2) **61.5±0.9**	266.1 **257.4±3.7**	(1) Correlation (2) Calorimetry	(1) 1995DEN (2) 2001LAG/DIO

2,2,2-tribromoacetic acid **Br**–$CBr_2C(O)OH$	60.8	254.4	Correlation	1995DEN
ethyl 2,2-dibromoacetate **Br**–$CHBrC(O)OC_2H_5$	62.9	263.2	Correlation	1995DEN
ethyl 2,2,2-tribromoacetate **Br**–$CBr_2C(O)OC_2H_5$	58.9	246.4	Correlation	1995DEN
diethyl 2-bromopropane-1,3-dioate **Br**–$CH(C(O)OEt)_2$	63.5	265.7	Correlation	1995DEN
diethyl 2,2-dibromopropane-1,3-dioate **Br**–$CBr(C(O)OEt)_2$	61.4	256.9	Correlation	1995DEN

5.4 C–I bonds

Table 5.4 C–I BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
cyanogen iodide **I**–CN	(1) 72.5±1.2 (2) **77.1**	303.3±5.0 **322.6**	(1) AP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1978DAY/GOW (2) 2002CRC
trifluoroiodomethane **I**–CF_3	(1) 52.6±1.1 (2) 53.5 (3) 54.4±0.5 (4) **54.3±0.3** (5) 53.9±1.3	220.1±4.6 223.8 227.6±2.1 **227.2±1.3** 225.5±5.4	(1) Kinetics (3) Kinetics (2) Kinetics (4) PIMS (5) Review	(1) 1975OKA/WHI (2) 1984AHO/WHI (3) 1991SKO/DYM (4) 1997ASH/RUS (5) 1998CHA
chloroiodomethane **I**–CH_2Cl	48.8±0.2	204.2±0.8	Kinetics	1996SKO/DYM

(continued)

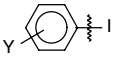
Table 5.4 (continued) C–I BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
diiodomethane **I**–CH_2I	(1) **51.9±2.0** (2) 50.6	**217.1±8.4** 211.7	(1) Derived from $\Delta_f H^o$ in ref. (2) Correlation	(1) 1993CAR/LAY (2) 1995DEN
iodomethane **I**–CH_3	57.1±0.5	238.9±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentafluoroiodoethane **I**–CF_2CF_3	(1) 51.2±1 (2) 52.3 (3) **52.4±0.5**	214.2±4.2 218.8 **219.2±2.1**	Kinetics	(1) 1976WU/ROD (2) 1984AHO/WHI (3) 1991SKO/DYM
1,1,1-trifluoro-2-iodoethane **I**–CH_2CF_3	(1) **56.3±1** (2) 52.9	**235.6±4.2** 221.3	(1) Iodination (2) Correlation	(1) 1973WU/ROD (2) 1995DEN
1-chloro-1,1,2-trifluoro-2-iodoethane **I**–CHFCClF2	48.3±0.5	203±2.0	Kinetics	1998SKO/DYM
1,1-difluoro-1-iodoethane **I**–CF_2CH_3	52±1	217.6±4.2	Review	1982MCM/GOL
1-fluoro-1,1-diiodoethane **I**–$CFICH_3$	52.1±1	218.0±4.2	Iodination	1976PIC/ROD
1-chloro-2-iodoethane **I**–CH_2CH_2Cl	54.2	226.8	Correlation	1995DEN
1-chloro-2-bromoethane **I**–CH_2CH_2Br	53.0	221.8	Correlation	1995DEN

pentafluoro-2-iodopropane $CF_3CF\mathbf{I}CF_3$	51.4	215.1	Kinetics	1984AHO/WHI
iodoethylene $\mathbf{I}–CH=CH_2$	61.9±1.0	259.0±4.2	Photo-fragmentation	1989CAO/ZHA
iodoethane $\mathbf{I}–C_2H_5$	55.8±1.5	233.5±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
3-iodo-1-propene $\mathbf{I}–CH_2CH=CH_2$	44.4±1.5	185.8±6.3	Derived from Δ_fH^o in ref.	1986PED/NAY
(Z)-1-iodo-1-propene $\mathbf{I}–CH=CHCH_3$	68.6±2	287.0±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
(E)-1-iodo-1-propene $\mathbf{I}–CH=CHCH_3$	67.0±2	280.3±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
1-iodopropane $\mathbf{I}–nC_3H_7$	56.6±1	236.8±4.2	Derived from Δ_fH^o in ref.	1986PED/NAY
2-iodopropane $\mathbf{I}–iC_3H_7$	(1) **56.1±1.5** (2) 53.4	**234.7±6.3** 223.4	(1) Derived from Δ_fH^o in ref. (2) Correlation	(1) 1986PED/NAY (2) 1995DEN
1,3-diiodopropane $\mathbf{I}–CH_2CH_2CH_2I$	54.4	227.6	Correlation	1995DEN
1-iodononafluorobutane $\mathbf{I}–C_4F_9$	49.2	205.8	Kinetics	1991SKO/DYM
2-iodobutane $\mathbf{I}–sC_4H_9$	54.1	226.4	Correlation	1995DEN

(continued)

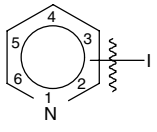
Table 5.4 (continued) C–I BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-iodo-2-methylpropane **I**–tC_4H_9	(1) **54.3±1.5**	**227.2±6.3**	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 52.1	218.0	(2) Correlation	(2) 1995DEN
1-iodo-3,3-dimethylpropane **I**–$CH_2(CH_3)_3$	55.7	233.0	Correlation	1995DEN
iodobenzene **I**–C_6H_5	65.0±1	272.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentafluoroiodobenzene **I**–C_6F_5	(1) 65.4±2	273.6±8.4	(1) Toluene carrier tech	(1) 1976KOM/KRE
	(2) <72.1	<301.7	(2) Electron capture detection	(2) 1989CHE/ALB
iodobenzene, substituted 				
Y = 2-F	65.9	275.7	Correlation	1995DEN
2-Cl	65.1	272.4		
2-Br	64.2	268.6		
2-I	63.6	266.1		
2-Me	65.7	274.9		
2-CF_3	63.2	264.4		
2-NH_2	66.7	279.1		
2-NO_2	65.6	274.5		
2-MeO	66.6	278.7		
2-Et	65.5	274.1		
2-EtO	66.7	279.1		

2-Ph	64.8	271.1		
2,6-Me_2	65.9	275.7		
iodocyclohexane **I**–c-C_6H_{11}	(1) **55.5±1.5**	**232.2±6.3**	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 54.3	227.2	(2) Correlation	(2) 1995DEN
benzyl iodide **I**–$CH_2C_6H_5$	(1) 45.4	190.0	(1) Shock wave	(1) 1990HIP/TRO
	(2) 43.9±2	183.7±8.4	(2) Derived from $\Delta_f H^o$ in ref.	(2) 1998NIST
	(3) **43.5±2**	**182.0±8.4**	(3) Derived from $\Delta_f H^o$ in ref.	(3) 2002VER/KRA
(2-iodoethyl)benzene **I**–$CH_2CH_2C_6H_5$	54.9	229.7	Correlation	1995DEN
1-iodonaphthalene **I**–1-naphthyl	(1) **65.6±2.5**	**274.5±10.5**	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 65.3	273.2	(2) Correlation	(2) 1995DEN
2-iodonaphthalene **I**–2-naphthyl	(1) 65.0±2.5	272.0±10.5	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY
	(2) 65.7	274.9	(2) Correlation	(2) 1995DEN
1-adamantyl iodide **I**–1-adamantyl	53.7	224.7	Correlation	1995DEN
iodoacetonitrile **I**–CH_2CN	44.7±2	187.0±8.4	Derived from $\Delta_f H^o$ in ref.	2000LAF/SZA
acetyl iodide **I**–$C(O)CH_3$	53.3±2	223.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
benzoyl iodide **I**–$C(O)C_6H_5$	50.7±2	212.1±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED

(continued)

Table 5.4 (continued) C–I BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
iodoacetic acid **I**–$CH_2C(O)OH$	(1) 51.2 (2) 47.2±0.6	214.2 197.8±2.7	(1) Correlation (2) Calorimetry	(1) 1995DEN (2) 2001LAG/DIO
3-iodopropanioc acid **I**–$CH_2CH_2C(O)OH$	54.5	228.0	Correlation	1995DEN
ethyl 2-iodoacetate **I**–$CH_2C(O)OC_2H_5$	51.9	217.1	Correlation	1995DEN
pyridine iodide 				
C–I at 2 site	63.1	264.0	Correlation	1995DEN
3	65.2	272.8		
4	64.9	271.5		

chapter six

Tabulated BDEs of O–X bonds

6.1 O–H bonds

6.1.1 O–H bonds in nonphenols

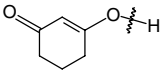
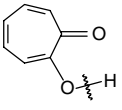
Table 6.1.1 O–H BDEs in Nonphenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
water	(1) **119.30±0.05**	**499.15±0.21**	(1) Recommend.	(1) 1994BER/ELL
HO–**H**	(2) 118.81±0.07	497.10±0.29	(2) Recommend.	(2) 2002RUS/WAG
$\Delta_f H^o(R)$ = 9.40±0.05 (39.33±0.21)	(3) 118.88±0.01	497.38±0.06	(3) Photolysis	(3) 2000HAR/HWA
methanol	(1) 104.4±1	436.8±4.2	(1) Kinetics	(1) 1974BAT/CHR
CH_3O–**H**	(2) 104.2±0.9	436.0±3.8	(2) Photoelectr.	(2) 1986MEO/SIE
$\Delta_f H^o(R)$ = 4.1±0.9	(3) **104.2±0.9**	**436.0±3.8**	(3) Recommend.	(3) 1994BER/ELL
(17.2±3.8)	(4) 104.9±0.7	439±3	(4) CID	(4) 1999DET/ERV
	(5) 104.6±0.7	437.7±2.8	(5) GPA, revised	(5) 2002ERV/DET
trifluoromethanol	(1) 109	456.1	(1) Pyrolysis	(1) 1982BAT/WAL
CF_3O–**H**	(2) 120±3	502.1±12.6	(2) FT-IR	(2) 1993WAL/HUR
$\Delta_f H^o(R)$ = –151.8±1.7 (–635.1±7.1)	(3) 124.7±3.6	521.7±15.1	(3) Flowing afterglow tech.	(3) 1996HUE/DUN
	(4) 117.5	491.6	(4) PIMS	(4) 1997ASH/APP
	(5) **118.8**	**497.1**	(5) Recommend.	(5) 2000REI/PRA
ethyn-1-ol HC≡CO–**H**	105.9±2.1	443.1	Photoelectr.	1983OAK/JON

(continued)

Table 6.1.1 (continued) O–H BDEs in Nonphenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
ethanol C_2H_5O–**H** $\Delta_f H^o(R)$ = –3.7±0.8 (–15.5±3.3)	(1) 104.2±1 (2) **104.6±0.8** (3) 103.0 (4) 105.2±1.2 (5) 104.7±0.8	436.0±4.2 **437.6±3.3** 431.0 440.0±5.0 438.1±3.3	(1) Pyrolysis (2) Recommend. (3) AOP (4) CID (5) GPA, revised	(1) 1974BAT/CHR (2) 1994BER/ELL (3) 1996BOR/LIU (4) 1999DET/ERV (5) 2002ERV/DET
vinyl alcohol CH_2=CHO–**H** $\Delta_f H^o(R)$ = 4.4±0.3 (18.4±1.3)	85	355.6	FT-ICR	2001BOU/CHA
1-propanol nC_3H_7O–**H** $\Delta_f H^o(R)$ = –7.2±2 (–30.1±8.4)	(1) 105.9±2 (2) 103.4±1	443.1±8.4 432.6±4.2	(1) Review (2) Pyrolysis	(1) 1973BEN/ONE (2) 1974BAT/CHR
2-propanol iC_3H_7O–**H** $\Delta_f H^o(R)$ = –12.5 (–52.3)	(1) 104.7±1 (2) 103.9 (3) 105.9±1.0 (4) **105.7±0.7**	438.1±4.2 434.7 443±4 **442.3±2.8**	(1) Pyrolysis (2) AOP (3) CID (4) GPA, revised	(1) 1974BAT/CHR (2) 1996BOR/LIU (3) 1999DET/ERV (4) 2002ERV/DET
1-butanol nC_4H_9O–**H** $\Delta_f H^o(R)$ = –15 (–62.8)	101.9±1	426.3±4.2	Pyrolysis	1974BAT/CHR
2-butanol sC_4H_9O–**H** $\Delta_f H^o(R)$ = –16.6 (69.5)	105.5±1	441.4±4.2	Pyrolysis	1974BAT/CHR
tert-butyl alcohol tC_4H_9O–**H**	(1) 105.1±1 (2) 105.5	439.7±4.2 441.4	(1) Pyrolysis (2) AOP	(1) 1974BAT/CHR (2) 1996BOR/LIU

$\Delta_f H^o(R) = -22.3$ (–93.3)	(3) 106.6±0.7 (4) 105.5 (5) **106.3±0.7**	446±3.0 441.4 **444.9±2.8**	(3) CID (4) PAC (5) GPA, revised	(3) 1999DET/ERV (4) 2000REI/PRA (5) 2002ERV/DET
neopentyl alcohol $tBuCH_2O$–**H**	102.3±1	428.0±4.2	Pyrolysis	1974BAT/CHR
benzyl alcohol $C_6H_5CH_2O$–**H** $\Delta_f H^o(R) = 25.6 \pm 3.0$ (107.1±12.6)	101.7	425.5	AOP	1996BOR/LIU
1,3-cyclohexadione 	92	384.9	AOP	1994BOR/SAT
tropolone 	88	368.2	AOP	1994BOR/SAT
acetic acid $CH_3C(O)O$–**H** $\Delta_f H^o(R) = -49.6 \pm 1$ (–207.5±4.2)	(1) 106.4 (2) 105.8±2	445.2 442.7	(1) Electrochem. (2) Review	(1) 1963EBE (2) 1973BEN/ONE
propanoic acid $C_2H_5C(O)O$–**H** $\Delta_f H^o(R) = -54.6 \pm 1$ (–228.4±6.4)	106.4±2	445.2	Review	1973BEN/ONE
butanoic acid $nC_3H_7C(O)O$–**H** $\Delta_f H^o(R) = -59.6 \pm 1$ (–249.4±4.2)	105.9±2	443.1	Review	1973BEN/ONE

(continued)

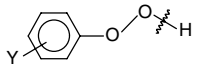
Table 6.1.1 (continued) O–H BDEs in Nonphenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
benzoic acid $C_6H_5C(O)O$–**H** $\Delta_f H^o(R) = -17.4\pm2$ (-72.8 ± 8.4)	105	439.3	AOP	1994BOR/SAT
hydroperoxide HOO–**H** $\Delta_f H^o(R) = 3.5$ (14.6)	(1) 87.2±1.0	364.8±6.4	(1) Laser magnetic resonance	(1) 1980HOW
	(2) **88.2±1.0**	**369.0±4.2**	(2) Review	(2) 1983SHU/BEN
	(3) 87.9±0.8	367.8±3.3	(3) GPA	(3) 1998LIT/RUS
	(4) 87.8±0.5	367.4±2.1	(4) Photoelectron spectra	(4) 2002RAM/BLA
methyl hydroperoxide CH_3OO–**H** $\Delta_f H^o(R) = 2.2\pm1.2$ (9.2 ± 5.0)	(1) **88.5±0.5**	**370.3±2.1**	(1) VLPP	(1) 1984KON/BEN(b)
	(2) 87.2	365	(2) Electrochem.	(2) 1996JON
trifluoromethyl hydroperoxide CF_3OO–**H**	91.5	383	Electrochem.	1996JON
fluoromethyl hydroperoxide CH_2FOO–**H**	90.6	379	Electrochem.	1996JON
trichloromethyl hydroperoxide CCl_3OO–**H**	92.3	386	Electrochem.	1996JON
dichloromethyl hydroperoxide $CHCl_2OO$–**H**	91.5	383	Electrochem.	1996JON
chloromethyl hydroperoxide CH_2ClOO–**H**	90.3	379	Electrochem.	1996JON

tribromomethyl hydroperoxide CBr_3OO–**H**	91.5	383	Electrochem.	1996JON
bromomethyl hydroperoxide CH_2BrOO–**H**	90.6	379	Electrochem.	1996JON
ethyl hydroperoxide C_2H_5OO–**H**	(1) 86.8 (2) 84.8±2.2	363 354.8	(1) Electrochem. (2) GPA	(1) 1996JON (2) 2001BLA/RAM
2-chloroethyl hydroperoxide $CH_3CHClOO$–**H**	90.1	377	Electrochem.	1996JON
2,2-dichloroethyl hydroperoxide CH_3CCl_2OO–**H**	91.5	383	Electrochem.	1996JON
1,1,1-trifluoro-2-chloroethyl hydroperoxide $CF_3CHClOO$–**H**	91.8	384	Electrochem.	1996JON
pentachloroethyl hydroperoxide C_2Cl_5OO–**H**	91.5	383	Electrochem.	1996JON
iso-propyl hydroperoxide iC_3H_7OO–**H**	85.1	356	Electrochem.	1996JON
allyl hydroperoxide CH_2=$CHCH_2OO$–**H** $\Delta_fH^o(R)$ = 21.2 (88.7)	(1) 89 (2) 86.8	372.4 363	(1) Photolysis (2) Electrochem.	(1) 1981RUI/BAY (2) 1996JON
tert-butyl hydroperoxide t-C_4H_9OO–**H**	(1) 89.4 (2) 82.2	374.0 344	(1) VPPR (2) Electrochem.	(1) 1983HEN/BEN (2) 1996JON

(continued)

Table 6.1.1 (continued) O–H BDEs in Nonphenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
	(3) **88.2**	**369.0**	(3) Review	(3) 1997BEN/COH
	(4) 85.0±2.0	355.6±8.4	(4) Photoelectr. spectroscopy	(4) 1998CLI/WEN
	(5) 84.2±2.1	352.3±8.8	(5) GPA	(5) 2001BLA/RAM
benzyl hydroperoxide $C_6H_5CH_2OO$–**H**	86.8	363	Electrochem.	1996JON
p-NO_2-benzyl hydroperoxide p-NO_2–$C_6H_4CH_2OO$–**H**	87.5	366	Electrochem.	1996JON
diphenylmethyl hydroperoxide $(C_6H_5)_2CHOO$–**H**	88.4	370	Electrochem.	1996JON
phenyl hydroperoxide, substituted 				
Y = H	91.8	384	Electrochem.	1996JON
p-Cl	92.0	385		
p-Me	91.5	383		
p-OH	91.3	382		
p-CN	92.1	385		
p-Ph	93.2	389		
p-CO_2	92.0	385		
methaneperoxycarboxylic acid $CH_3C(O)OO$–**H**	92.3	386	Electrochem.	1996JON

2,2-dichloro-2-hydro-peroxyethane $CCl_2(CN)OO$–**H**	91.8	384	Electrochem.	1996JON
hydroperoxymethan-ol $OHCH_2OO$–**H**	88.0	368	Electrochem.	1996JON
2-hydroperoxypropan-ol $(CH_3)_2C(OH)OO$–**H**	86.5	362	Electrochem.	1996JON
1-hydroperoxyacetone $CH_3C(O)CH_2OO$–**H**	88.0	368	Electrochem.	1996JON
α-CO_2^--methyl hydroperoxide $(CO_2^-)CH_2OO$–**H**	87.5	366	Electrochem.	1996JON
2-hydroperoxyethanenitrile $(CN)CH_2OO$–**H**	89.9	376	Electrochem.	1996JON
α-CO_2^--chloromethyl hydroperoxide $(CO_2^-)CHClOO$–**H**	90.3	378	Electrochem.	1996JON
α-CO_2^--dichloromethyl hydroperoxide $(CO_2^-)CCl_2OO$–**H**	90.3	378	Electrochem.	1996JON
2,2-dichloro-2-hydroperoxy-ethanenitrile $(CN)CCl_2OO$–**H**	91.8	384	Electrochem.	1996JON
naphth-1-yl hydroperoxide 1-$C_{10}H_7OO$–**H**	93.9	393	Electrochem.	1996JON

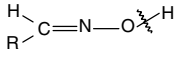
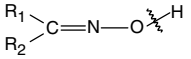
(continued)

Table 6.1.1 (continued) O–H BDEs in Nonphenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
naphth-2-yl hydroperoxide 2-$C_{10}H_7OO$–**H**	93.2	390	Electrochem.	1996JON
9-anthracenyl hydroperoxide 9-$C_{14}H_9OO$–**H**	93.9	393	Electrochem.	1996JON
in enols R_1R_2C=CR(O**H**) Mes = mesityl				
R_1 R_2 R			AOP	1997BOR/ZHA
Mes Mes H	82.2	343.9		
Mes Mes Mes	82.6	345.6		
Mes Mes Me_3Si	82.4	344.8		
Mes Mes Ph	79.9	334.3		
Mes Mes iPr	78.6	328.9		
Mes Mes tBu	78.3	327.6		
Mes Ph Mes	83.7	350.2		
Me_5C_6 Me_5C_6 H	82.3	344.3		
H H Me	83	347.3		
nitrous acid **H**–ONO $\Delta_f H^o(R)$ = 7.91 (33.09)	78.3±0.5	327.6±2.1	Review	1976BEN
nitric acid **H**–ONO_2 $\Delta_f H^o(R)$ = 17.0 (71.1)	104±1	435.1±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimeylsilaethanol **H**–$OSiMe_3$	118.3	495	Derived	1998BEC/WAL

6.1.2 O–H bonds in oximes and hydrolamines

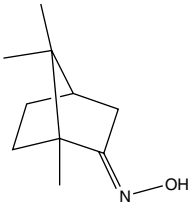
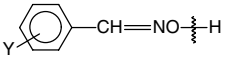
Table 6.1.2 O–H BDEs in Oximes and Hydrolamines

The broken bonds (**boldface =** dissociated group)		BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
oximes					
					
R = Me		98.2	410.9	AOP	1992BOR/JI
Et		98.1	410.5		
CH_3CO		89.6	374.9		
PhCO		88.9	372.0		
NH_2		88.8	371.5		
oximes					
					
R_1 = Me	R_2 = Me	(1) 95.8 (2) 94.1	400.8 393.7	(1) AOP (2) Correlation	(1) 1992BOR/JI (2) 2000DEN/DEN
Et	Et	(1) 92.3 (2) 90.6	386.2 379.1		
iPr	rPr	(3) 87.7 (2) 86.0	366.9 359.8	(3) AOP	(3) 1995BOR/ ZHA(b)
Me	tBu	(3) 91.1	381.2		
iPr	tBu	(2) 84.3 (4) 84.3 (5) 86.0	352.7 352.7 359.8	 (4) EPR (5) AOP	 (4) 1973MAH/MEN (5) 1996BOR/LIU
tBu	tBu	(2) 80.9 (3) 84.2 (4) 80.9 (5) 82.6	338.5 352.3 338.5 345.6		
tBu	adamantyl	(3) 81.7 (4) 80.0	341.8 334.7		
tBu	c-C_5H_9	(3) 90.7	379.5		

(continued)

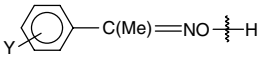
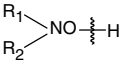
Table 6.1.2 (continued) O–H BDEs in Oxides and Hydrolamines

The broken bonds (**boldface =** dissociated group)		BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
Ph	Ph	(1) 89.0	372.4		
$PhCH_2$	$PhCH_2$	(1) 89.1	372.8		
Me	Et_2NCH_2	(1) 91.4	382.4		
Me	NH_2	(1) 86.7	362.8		
Ph	NH_2	(1) 86.9	363.6		
cyclohexanone, oximes c-$C_5H_{10}C$=NO–**H**		(1) 90.3 (2) 88.6	377.8 370.7	(1) AOP (2) Correlation	(1) 1995BOR/ZHA(b) (2) 2000DEN/DEN
cycloundercanane, oximes c-$C_{11}H_{22}C$=NO–**H**		90.3	377.8	AOP	1992BOR/JI
oximes, substituted					
(Z)-PhCH=NO–**H**		90.2	377.4	AOP	1995BOR/ZHA(b)
(E)-PhCH=NO–**H**		86.9	363.6		
(Z)-p-MeC_6H_4CH=NO–**H**		89.0	372.4		
(E)-p-MeC_6H_4CH=NO–**H**		86.5	361.9		
(Z)-p-$MeOC_6H_4$CH=NO–**H**		89.9	376.1		
(E)-p-$MeOC_6H_4$CH=NO–**H**		87.5	366.1		
(Z)-m-$NO_2C_6H_4$CH=NO–**H**		88.6	370.7		
(E)-m-$NO_2C_6H_4$CH=NO–**H**		86.9	363.6		
(Z)-p-$NO_2C_6H_4$CH=NO–**H**		88.0	368.2		
(Z)-PhCHCHCH=NO–**H**		88.6	370.7		
(Z)-CH_3C(Ph)=NO–**H**		91.1	381.2		
(E)-CH_3C(Ph)= NO–**H**		89.4	374.0		
(Z)-$Me_2NCH_2C(CH_3)$=NO**H**		92.0	384.9		
(E)-Me_2NCH_2C(Ph)=NO**H**		88.5	370.3		
(Z)-(c-C_4H_8N)CH_2C(Ph)=NO**H**		88.6	370.7		
(E)-Me_2NCH_2C(Ph)=NO**H**		87.6	366.5		

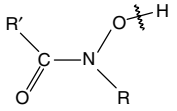
(Z)-(c-C_4H_8N)CH_2C(Ph)=NO**H**	89.1	372.8		
(E)-$Me_2NCH_2CH_2C$(Ph)=NO**H**	88.7	371.1		
2-(hydroxyimino)-1,7, 7-trimethylbicyclo [2.2.1]-heptane 	88.1	368.6	AOP	1995BOR/ZHA(b)
norcamphor, oximes R=NO–**H**	87.6	366.5	AOP	1995BOR/ZHA(b)
fluorene, oximes Fl=NO–**H**	87.5	366.1	AOP	1992BOR/JI
(hydroxyimino)-2, 7-dibromo-fluorenylmethane 2,7-BrFl=NO–**H**	89.6	375.3	AOP	1992BOR/JI
(hydroxyimino)-2-$PhSO_2$- fluorenylmethane 2-$PhSO_2$Fl=NO–**H**	89.0	372.4	AOP	1992BOR/JI
oximes, substituted 				
Y = H	88.1	368.6	AOP	1998BOR/ZHA
p-Cl	87.8	367.4		
p-Br	87.6	366.5		
p-MeO	87.8	367.4		

(continued)

Table 6.1.2 (continued) O–H BDEs in Oxides and Hydrolamines

The broken bonds (**boldface =** dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
p-Me	88.0	368.2		
p-CF_3	87.9	367.8		
p-CN	87.8	367.4		
m-NO_2	88.6	370.7		
p-NO_2	88.4	369.9		
oximes, substituted 				
Y = H	88.4	369.9	AOP	1998BOR/ZHA
p-Cl	89.0	372.4		
p-Br	89.0	372.4		
p-Me	89.0	372.4		
p-MeO	88.9	372.0		
p-CF_3	88.9	372.0		
p-CN	88.8	371.5		
p-NO_2	88.8	371.5		
hydroxylamines, substituted 				
R_1 = CF_3 R_2 = CF_3	(1) 85.3	356.9	(1) EPR	(1) 1984DOB/ING
Et Et	(2) 69.5	290.8	(2) Kinetics	(2) 1978CAC/LIS
	(3) 75.9	317.6	(3) AOP	(3) 1996BOR/LIU
	(4) 72.8	304.5	(4) Correlation	(4) 2000DEN/DEN
tBu tBu	(3) 68.2	285.3		
	(5) <69.6	291.2	(5) EPR	(5) 1973MAH/MEN

hydroxamic acid, substituted

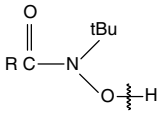


R′ = iPr	R = Ph	(1) 79.3 (2) 81.2	331.8 339.7	(1) EPR (2) AOP	(1) 1990PER/BER (2) 1996BOR/LIU
tBu	Ph	(1) 78.0 (2) 79.9	326.4 334.3		
Ph	Ph	(2) 84.1	351.9		
Ph	p-BrC_6H_4	(2) 84.0	351.5		
Ph	p-$CN–C_6H_4$	(2) 84.2	352.3		
tBu	p-$O_2N–C_6H_4$	(1) 80.2	335.6		
tBu	p-$MeO–C_6H_4$	(1) 75.9	317.6		
tBu	n-$C_{10}H_{21}$	(1) 75.8	317.1		
tBu	$N(CH_2)_5$	(1) 74.4	311.3		
3,5-(tBu)–C_6H_3	Ph	(1) 80.5	336.8		

hydroxylamines, substituted
R(tBu)NO–**H**

R = $iPrCH_2C(O)$	75.6	316.5	Correlation	2000DEN/DEN
$PhCH_2CH_2C(O)$	76.1	318.6		
$CH_3(CH_2)_9C(O)$	75.8	317.2		
C(O)CHCHPh	76.8	321.4		
4-$NO_2C_6H_4$	80.2	335.6		
4-$MeOC_6H_4C(O)$	73.5	307.7		

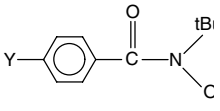
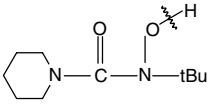
N-(tert-butyl)-N-hydroxy-
carboxamide, substituted



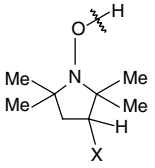
R = PhCH=CH	76.8	321.3	EPR	1983JEN/PER
$PhCH_2CH_2$	76.2	318.8		

(continued)

Table 6.1.2 (continued) O–H BDEs in Oximes and Hydrolamines

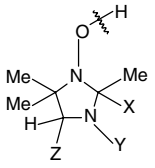
The broken bonds (**boldface =** dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$CH_3(CH2)_9$	75.8	317.1		
$(CH_3)_2CHCH_2$	75.6	316.3		
	74.4	311.3		
N-(tert-butyl)-N-hydroxy-benzamide, substituted 				
Y = H	77.2	323.0	EPR	1983JEN/PER
Ph	76.7	320.9		
NO_2	79.4	332.2		
MeO	75.1	314.2		
hydroxy-N-piperidine, substituted 	74.4	311.1	Correlation	2000DEN/DEN
phenylamine, substituted $(4\text{-R–}C_6H_4)_2NO–\mathbf{H}$				
R = MeO	71.8	300.3	Correlation	2000DEN/DEN
t-Bu	70.9	296.5		

1-hydroxy-pyrrolidine, substituted



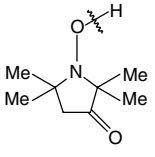
X = $CONH_2$	69.6	291.0	Correlation	2000DEN/DEN
C(O)OH	69.3	290.1		
OH	69.1	289.1		

1-hydroxy-tetrahydro-imidazole



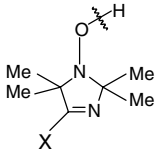
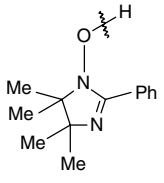
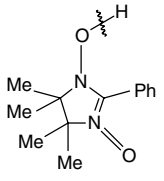
X	Y	Z				
Me	OH	H	71.9	300.9	Correlation	2000DEN/DEN
Me	Me	H	69.5	290.8		
Me	Me	Me	68.6	286.9		
Me	Me	p-FC_6H_4	69.8	292.0		
Me	Me	p-MeC_6H_4	69.5	290.7		
Me	Me	Ph	69.9	292.6		
Me	H	PhC(O)CH=	71.4	298.7		

1-hydroxy-pyrrolidine, substituted	71.4	298.7	Correlation	2000DEN/DEN

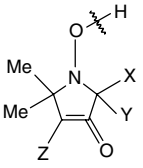


(continued)

Table 6.1.2 (continued) O–H BDEs in Oxides and Hydrolamines

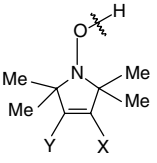
The broken bonds (**boldface =** dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
hydroimidazole, substituted 				
X = Me	70.6	295.2	Correlation	2000DEN/DEN
iPr	70.5	294.9		
CCl_3	71.0	296.9		
Ph	70.3	294.2		
p-FC_6H_4	70.8	296.1		
p-ClC_6H_4	70.5	294.9		
$C(O)NH_2$	71.0	296.9		
$CH_3C_6H_4$	71.0	296.9		
C(O)Me	71.0	296.9		
CH=N–tBu	70.5	294.8		
CH=NOH	70.8	296.1		
hydroimidazole, substituted 	74.6	312.2	Correlation	2000DEN/DEN
hydroimidazole, substituted 	71.0	297.1	Correlation	2000DEN/DEN

2,5-dihydrioimidazole, substituted



X	Y	Z				
Me	NMeOH	Ph	74.1	310.0	Correlation	2000DEN/DEN
Me	Me	Me	73.1	305.8		
Me	Me	$BrCHCH_3$	73.1	305.8		
Me	Me	p-BrC_6H_4	73.1	305.8		
Me	Me	$CHBr_2$	74.4	311.1		
Me	Me	p-ClC_6H_4	73.2	306.3		
Me	Me	$CHCl_2$	74.0	309.8		
Me	Me	p-FC_6H_4	73.1	305.8		
Me	NHMe	Ph	74.0	309.8		
Me	Me	CH_2Br	73.2	306.3		
Me	Me	p-$MeOC_6H_4$	72.5	303.4		
Me	Me	p-MeC_6H_4	72.6	303.6		
Me	Me	Ph	72.8	304.5		

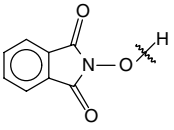
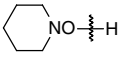
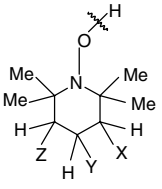
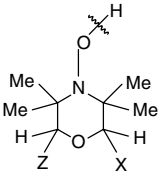
2,5-dihydropyrrole, substituted

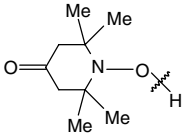
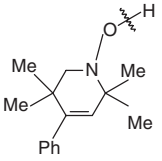
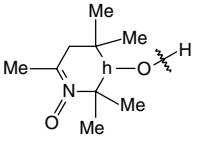
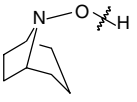
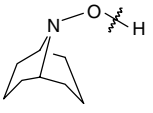


X = Cl	Y = H	70.1	293.1	Correlation	2000DEN/DEN
COMe	H	70.3	294.3		
$CONH_2$	H	70.1	293.1		
C(O)OH	H	69.6	291.0		
C(O)OMe	H	70.1	293.1		
Br	Br	70.2	293.7		

(continued)

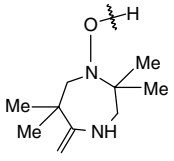
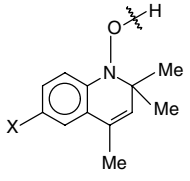
Table 6.1.2 (continued) O–H BDEs in Oximes and Hydrolamines

The broken bonds (**boldface =** dissociated group)		BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
C(O)OMe	Br	70.1	293.1		
COMe	Br	70.4	294.5		
N-hydroxyphthalimide 		>86	>359.8	EPR	2002MIN/PUN
piperidinol 		77.0	322.2	AOP	1996BOR/LIU(b)
piperdin-1-ol, substituted 					
X	Y	Z			
H	H	H	(1) 69.6 (2) 69.7 (3) 71.2	291.2 291.6 297.7	(1) EPR (2) AOP (3) Correlation	(1) 1973MAH/MEN (2) 1996BOR/LIU (3) 2000DEN/DEN
H	PhC(O)O	H	(3) 71.2	297.7		
H	OH	H	(3) 72.2	302.2		
1-hydroxy-piperidine, substituted 					

X = Cl	H	73.6	307.9	Correlation	2000DEN/DEN
Br	H	72.5	303.4		
1-hydroxy-piperidn-4-one, substituted 		71.8	300.4	EPR	1973MAH/MEN
1-hydroxy-1,2,5, 6-tetra-hydropyridine, substituted 		70.7	295.9	Correlation	2000DEN/DEN
1-hydroxy-1,2,5, 6-tetra-hydropyrimidine, substituted 		73.8	308.8	Correlation	2000DEN/DEN
7-aza-bicyclo[2.2.1] heptan-7-ol 		(1) 77.0 (2) 78.0	322.2 326.4	(1) EPR (2) AOP	(1) 1973MAH/MEN (2) 1996BOR/LIU
9-azabicyclo[3.3.1] nonane-9-ol 		76.2	318.8	EPR	1973MAH/MEN

(continued)

Table 6.1.2 (continued) O–H BDEs in Oximes and Hydrolamines

The broken bonds (**boldface =** dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
hydroxydiazacycloheptane, substituted 	72.7	304.3	Correlation	2000DEN/DEN
1,2-dihydroquinoline, substituted 				
X = $C(CF_3)2OH$	70.5	294.9	Correlation	2000DEN/DEN
CPh3	69.2	289.5		

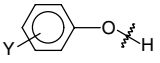
6.1.3 O–H bonds in phenols

Table 6.1.3 O–H BDEs in Phenols

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
phenol	(1) 89.5±1	374.5±4.2	(1) VLPP	(1) 1989SUR/KAF
PhO–**H**	(2) 88.3±1.5	369.4±6.3	(2) SPST	(2) 1990WAL/TSA
$\Delta_f H^o(R)$ = 12.9±1.5 (54±6)	(3) **90.4±1** in sol.	**378.2±4.2** in sol.	(3) AOP	(3) 1996BOR/LIU
	(4) **88.0±1.5** in gas	**368.2±6.3** in gas	(4) Recommend.	(4) 1996TSA
	(5) 87.3±1.5 in gas	365.3±6.3 in gas	(5) PAC	(5) 1997WRI/CAR

pentafluorophenol C_6F_5O–**H**	85.5	357.7	Correlation	2000DEN/DEN

phenols, substituted



Y = p-F	(1) 91.2 (3) 87.4±0.5 (5) 84.5 (14) 87.2	381.6 365.7±2.1 353.5 365.0	(1) AOP (2) AOP (3) Pulse radiolysis	(1) 1990ARN/AMA (2) 1991BOR/CHE(b) (3) 1990LIN/SHE
m-F	(14) 89.0	372.7	(4) EPR	(4) 1996LUC/PED
o-F	(14) 86.3	361.0	(5) Electrochem.	(5) 1992PAR
p-Cl	(1) 93.4 (2) 90.3 (3) 87.6±0.5 (8) 91.1 (12) 90.9	390.8 378.0±2.0 366.5±2.1 381.0 380.3	(6) EPR	(6) 1973MAH/MEN
m-Cl	(2) 91.8 (14) 88.4	384.1 369.9	(7) PAC	(7) 2001SIL/MAT
o-Cl	(2) 90.0 (14) 86.1	376.6 359.9	(8) AOP	(8) 1997ZHU/ZHA
p-Br	(2) 90.7 (3) 88.1±0.5 (5) 85.2 (8) 91.3 (14) 89.0	379.5 368.6±2.1 356.5 382.0 372.3	(9) AOP	(9) 1994ZHA/BOR
o-Br	(14) 86.4	361.8	(10) Electrochem.	(10) 1991PAR/HAN
p-I	(3) 87.9±0.3 (5) 85.1	367.8±1.3 356.1	(11) EPR	(11) 1994LUC/PED
p-Me	(1) 87.2 (2) 88.7 (3) 86.1±0.5 (4) 88.2±0.6 (8) 89.4	364.8 371.1 360.2±2.1 369.0±2.5 374.0	(12) AOP	(12) 1996BOR/LIU
m-Me	(2) 89.4 (14) 87.6	374.0 366.7	(13) Electrochem.	(13) 1975MAH/DAR

(continued)

Table 6.1.3 (continued) O–H BDEs in Phenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
o-Me	(2) 88.2	369.0	(14) Correlation	(14) 2000DEN/DEN
	(12) 90.0	376.6		
	(14) 86.1	359.9		
p-CN	(1) 93.1	389.5		
	(2) 94.2	394.1		
	(3) 92.9±0.7	388.7±2.9		
	(5) 90.1	377.0		
	(8) 94.9	397.0		
m-CN	(2) 93.9	392.9		
	(14) 89.3	373.6		
o-CN	(14) 88.0	368.1		
p-NO_2	(1) 93.8	392.5		
	(2) 94.7	396.2		
	(3) 94.2±1.4	394.1±5.9		
	(5) 91.3	382.0		
	(8) 95.4	399.0		
m-NO_2	(2) 94.3	394.6		
	(14) 87.7	366.9		
o-NO_2	(14) 86.9	363.4		
p-MeO	(1) 86.3	361.1		
	(3) 82.6±0.5	345.6±2.1		
	(4) 82.8±0.2	346.4±0.8		
	(8) 85.1	356.0		
	(13) 84.0	351.5		
m-MeO	(2) 90.2	377.4		
	(12) 90.8	379.9		
	(14) 88.4	369.8		
o-MeO	(2) 86.0	359.8		
	(14) 84.2	352.1		
p-O^-	(2) 73.0	305.4		
	(3) 72.4	302.9		
p-OH	(2) 81.5	341.0		
	(3) 80.2	335.6		
	(8) 82.2	344.0		
	(13) 84.6	354.0		
	(14) 84.1	352.0		

m-OH	(2) 90.9	380.3
	(14) 88.2	369.1
o-OH	(14) 81.2	339.6
p-NH_2	(2) 77.3	323.4
	(3) 75.5	315.9
	(8) 77.9	326.0
	(14) 80.8	338.1
m-NH_2	(2) 88.0	368.2
	(8) 88.0	368.0
	(14) 87.8	367.2
o-NH_2	(14) 85.3	356.7
p-CF_3	(2) 95.3	398.7
	(8) 95.8	401.0
	(14) 91.4	382.4
m-CF_3	(2) 93.8	392.5
	(14) 92.2	385.7
p-tBu	(2) 88.7	371.1
	(4) 85.3±0.5	356.9±2.1
	(8) 89.4	374.0
	(13) 86.5	361.9
	(14) 86.1	360.1
o-tBu	(14) 84.6	354.0
p-Ph	(2) 87.6	366.5
	(8) 88.2	369.0
	(13) 85.0	355.6
	(14) 88.1	368.7
o-Ph	(14) 86.5	361.9
o-C_2H_3	(14) 85.8	358.9
p-CH_2OH	(14) 85.7	358.7
p-C(O)OH	(14) 88.8	371.7
p-$MeCO_2$	(1) 88.9	372.0
m-$EtCO_2$	(13) 89.9	376.1
	(14) 90.7	379.4
p-Me_2N	(2) 80.3	336.0
	(3) 74.1	310.0
	(8) 79.8	334.0
	(14) 78.6	328.9
m-Me_2N	(2) 87.9	367.8
	(14) 86.2	360.6

(continued)

Table 6.1.3 (continued) O–H BDEs in Phenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
p-$MeSO_2$	(2) 95.0	397.5		
	(8) 95.6	400.0		
m-$MeSO_2$	(2) 92.3	386.2		
	(14) 90.7	379.5		
p-MeCO	(2) 92.8	388.3		
	(3) 90.3±0.5	377.8±2.1		
	(5) 87.5	366.1		
	(8) 93.5	391.0		
	(14) 88.8	371.6		
m-MeCO	(2) 91.8	384.1		
	(14) 90.0	376.5		
o-MeCO	(14) 86.8	363.0		
p-PhCO	(2) 92.5	387.0		
	(8) 93.2	390.0		
	(14) 90.8	379.9		
p-COO^-	(3) 89.9±0.5	376.1		
	(5) 87.1	364.4		
o-$(CH_2)_3CHO$	(14) 86.9	363.6		
p-BuO	(14) 83.1	347.8		
phenols, disubstituted	(2) 93.9	392.9	(2) AOP	(2) 1991BOR/CHE(b)
3,5-Cl_2	(14) 92.3	386.2		
3,5-Me_2	(2) 89.1	372.8	(4) EPR	(4) 1996LUC/PED
	(8) 88.2	369.0		
	(12) 89.7	375.3		
	(14) 87.2	364.7		
2,3-Me_2	(14) 85.0	355.5	(7) PAC	(7) 2001SIL/MAT
2,4-Me_2	(14) 86.2	360.5	(8) AOP	(8) 1997ZHU/ZHA
2,6-Me_2	(2) 85.5	357.7	(10) Electrochem.	(10) 1991PAR/HAN
	(4) 84.5±0.4	353.5±1.7		
	(8) 87.2	365.0		
	(14) 84.8	354.6		
3,4-Me_2	(14) 84.8	354.6	(12) AOP	(12) 1996BOR/LIU

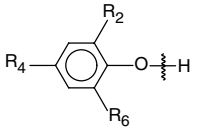
2-Me-4-tBu	(14) 86.0	359.9	(13) Electrochem.	(13) 1975MAH/DAR
2-tBu-4-Me	(14) 86.2	360.5	(14) Correlation	(14) 2000DEN/DEN
2,6-tBu_2 (also see Table 6.1.4)	(2) 82.1 (4) 82.8±0.2 (8) 82.7 (13) 85.1 (14) 82.8	343.5 346.4±0.8 346.0 356.1 346.4		
2,4-tBu_2	(14) 85.9	359.5		
3,5-tBu_2	(4) 86.6±0.3 (7) 90.3±0.5 (13) 86.9 (14) 86.6	362.3 377.8 363.6 362.4		
2,6-$(MeO)_2$	(4) 83.2±0.2	347.9		
3,5-$(MeO)_2$	(4) 86.7±0.3	362.8		
2-OH-4-tBu	(14) 81.8	342.4		
2-Me-4-OH	(14) 83.6	349.8		
2-tBu-4-MeO	(14) 82.1	343.4		
phenols, trisubstituted	(2) 93.1	389.5	(2) AOP	(2) 1991BOR/CHE(b)
3,4,5-Cl_3	(14) 91.4	382.4		
2,4,5-Me_3	(14) 85.3	356.8	(6) EPR	(6) 1973MAH/MEN
2,4,6-tBu_3 (also see Table 6.1.4)	(6) 81.2 (8) 82.2 (9) 82.6 (11) 81.2±0.1 (18) 81.3	339.7 344 345.6 339.7±0.4 340.2	(8) AOP (9) AOP (11) EPR	(8) 1997ZHU/ZHA (9) 1994ZHA/BOR (11) 1994LUC/PED
2,4-tBu_2–6-Me	(14) 85.1	355.9		
2,6-Me_2–4-Cl	(14) 84.0	351.4	(14) Correlation	(14) 2000DEN/DEN
3,5-Me_2–4-$CH_2C(O)OH$	(14) 83.7	350.3	(15) EPR	(15) 1996LUC/PED
2,6-Me_2–4-CN	(14) 84.6	354.0		
2,6-Me_2–4-NH_2CH_2	(14) 83.2	348.1	(16) EPR	(16) 2002LUC/MUG
2-OH–3,5-tBu_2	(14) 81.3	340.3	(18) EPR	(18) 2000PED/COR

(continued)

Table 6.1.3 (continued) O–H BDEs in Phenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-OH–3,6-tBu_2	(14) 81.1	339.5		
2,3-MeO–4-OH	(14) 82.2	343.8		
2,3-Me_2–4-MeO	(14) 79.2	331.4		
2-S$(CH_2)_2$ CN–4-Me–6-MePhCH	(14) 83.1	347.5		
2-Me–4-NH_2CH_2–6-tBu	(14) 83.8	350.6		
3,6-tBu_2–4-Me	(7) 80.5±0.9 (11) 80.7±0.3	336.8 337.6		
2-tBu–4,6-Me_2	(14) 85.1	355.8		
1,3-tBu_2–5-OH	(15) 79.3±0.3 (16) 80.7±0.3	331.8 337.6		
2,5-t-pentyl–4-OH	(16) 80.8±0.2	338.1±0.8		
4-C_3H_7–2,5-di-OH (propyl gallate)	(16) 82.6±0.3	345.6±1.3		
4-C_8H_{17}–2,5-di-OH (octyl gallate)	(16) 82.5±0.3	345.2±1.3		

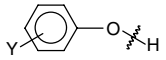
phenols, substituted



R_2	R_4	R_6	in sol.	in gas	in sol.	in gas		
H	H	H	(1) 89.2	87.3	373.2	365.3	(1) PAC	(1) 1995WAY/LUS
tBu	tBu	tBu	(2) 83.2	81.2	348.1	339.7	(2) Calorimetry	(2) 1989MAH/FER
tBu	Me	tBu	(3) 81.6 (4) 82.7 (5) 79.7	79.6 80.7	341.4 346.0 333.5	333.0 337.6	(3) PAC (4) EPR (5) EPR	(3) 1996WAY/LUS (4) 1994LUC/PED (5) 2000PED/COR
Me	Me	Me	(1) 83.8	81.8	350.6	342.3		

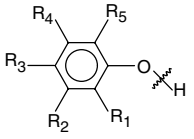
Me	MeO	Me	(3) 79.2	77.2	331.4	323.0		
			(4) 79.6	77.6	333.0	324.7		
tBu	t-Bu	H	(3) 84.1	82.1	351.9	343.5		

phenols, substituted



Y = H	in sol.	in gas	in sol.	in gas		
2-MeO	(1) 89.2	86.2	373.2	360.7	(1) PAC	(1) 1999HEE/KOR
2,6-$(MeO)_2$	(1) 88.6	86.6	370.7	362.3		
2,4-$(MeO)_2$	(1) 81.9	79.7	342.7	333.5		
2,4,6-$(MeO)_3$	(1) 83.5	81.5	348.4	341.0		
4-MeO	(1) 78.9	76.9	330.1	321.7		
	(2) 83.8	81.4	350.6	340.6		(2) 1996WAY/LUS

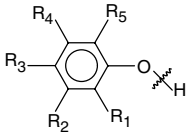
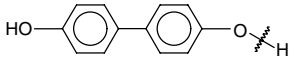
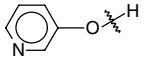
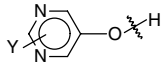
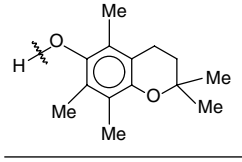
phenols, tetrasubstituted



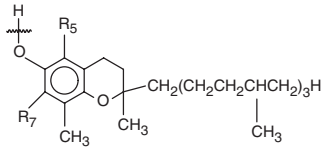
$R_1 = R_4 = R_5 = Me$ $R_2 = H$, $R_3 = MeO$	(1) 79.2±0.2	331.4±0.8	(1) EPR	(1) 1996LUC/PED
$R_1 = R_2 = R_4 = R_5 = Me$ $R_3 = H$	(4) 83.1	347.8	(2) EPR	(2) 1991COR/COL
$R_1 = R_2 = R_3 = R_5 = Me$ $R_4 = H$	(4) 83.9	351.2	(3) EPR	(3) 2002LUC/MUG
			(4) Correlation	(4) 2000DEN/DEN
$R_2 = R_5 = H$, $R_3 = OH$ $R_1 = R_4 = CMe_2Et$	(3) 80.8±0.2	338.1±0.8		
$R_1 = R_5 = OH$, $R_2 = R_4 = H$ $R_3 = C(O)OC_3H_7$	(3) 82.6±0.3	345.6±1.3		
$R_1 = R_5 = OH$, $R_2 = R_4 = H$ $R_3 = C(O)OC_8H_{17}$	(3) 82.5±0.3	345.2±1.3		
$R_1 = R_2 = R_4 = Me$ $R_3 = OH$, $R_5 = H$	(4) 82.4	344.7		

(continued)

Table 6.1.3 (continued) O–H BDEs in Phenols

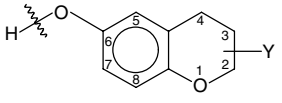
The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
phenols, pentasubstituted 				
$R_1 = R_2 = R_4 = R_5 = Me$ $R_3 = MeO$	(1) 81.9±0.2 (2) 78.0±0.1	342.7 326.4	(1) EPR (2) EPR	(1) 1996LUC/PED (2) 1991COR/COL
$R_1 = R_2 = R_3 = R_4 = R_5 = Me$	(3) 81.4	340.5	(3) Correlation	(3) 2000DEN/DEN
4,4′-dihydroxybiphenyl 	(1) 85.2 (2) 85.5	356.5 357.7	(1) Electrochem. (2) Pulse radiolysis	(1) 1975MAH/DAR (2) 2001DAS
3-hydroxypyridine 	95	397.5	AOP	1993BOR/SIN
5-pyrimidinols 				
Y = H	(1) 91.1	381.2	(1) Estimated by exp.	2001PRA/DIL
o-CH_3 o-CH_3 p-CH_3	(2) 85.2±0.5	356.5±2.1	(2) EPR	
o-tBu o-tBu p-CH_3	(2) 84.10±0.25	351.87±1.05		
o-CH_3 o-CH_3 p-$N(CH_3)_2$	(2) 78.16±0.25	327.02±1.05		
chroman-6-ol, substituted 	78.3±0.2	327.6±0.8	EPR	1996LUC/PED

α-tocopherol



$R_5 = R_7 = CH_3$ (vitamin E)	(1) 80.4	336.4	(1) Estimated by rate constants	(1) 1985BUR/DOB
	(2) 78.9	330.1	(2) EPR	(2) 1992JAC/HOS
	(3) 78.9	330.1	(3) EPR	(3) 1994LUC/PED
	(4) 80.9±1 in sol.	338.5	(4) AOP	(4) 1996BOR/LIU
	(5) **79.3** in sol.	**331.8**	(5) APC	(5) 1996WAY/LUS
	(5) **77.3** in gas	**323.4**		
δ-tocopherol $R_5 = R_7 = H$	(5) 82.2 in sol.	343.9	(6) Correlation	(6) 2000DEN/DEN
	(5) 80.2 in gas	335.6		
	(6) 81.9	342.8		
β-tocopherol $R_5 = CH_3$, $R_7 = H$	(6) 80.2	335.6		
γ-tocopherol $R_5 = H$, $R_7 = CH_3$	(6) 80.1	335.1		

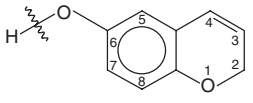
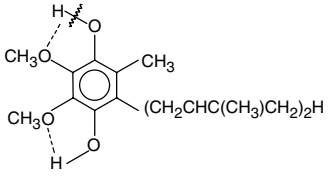
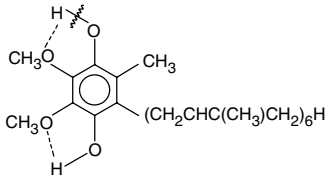
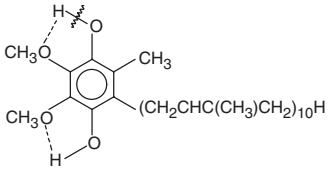
chroman, substituted



Y = 5,7,8-trimethyl	79.1	331.0	Correlation	2000DEN/DEN
2,4,5,7-tetramethyl	78.0	326.4		
2,5,7,8-tetramethyl-2-COOH	78.6	328.9		
2,5,7,8-tetramethyl-2-$CH_2CH_2C(O)COOH$	78.7	329.1		
2,5,7,8-tetramethyl-2-CH_2COOH	79.7	329.3		
2,5,7,8-tetramethyl-2-CH_3O	80.0	334.7		
2,5,7,8-tetramethyl-2 $CH_2CH_2C(O)OCH_3$	78.8	329.7		

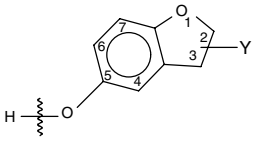
(continued)

Table 6.1.3 (continued) O–H BDEs in Phenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,2,5,7,8-pentamethyl	78.5	328.4		
2,5,7,8-tetramethy l-2- CH_2OH	79.1	331.0		
2H-chromene, substituted 2,2,5,7,8-pentamethyl 	79.2	331.5	Correlation	2000DEN/DEN
ubiquinol-2 	82.3	344.3	Correlation	2000DEN/DEN
ubiquinol-6 	82.3	344.3	Correlation	2000DEN/DEN
ubiquinol-10 	80.5 in sol. 78.5 in gas	336.8 in sol. 328.4 in gas	Correlation	1999HEE/KOR

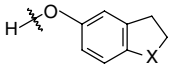
5,7-dimethy-tocol, DMT RO–**H**	79.7	333.5	PAC	2000DEN/DEN

dihydrobenzofuran, substituted



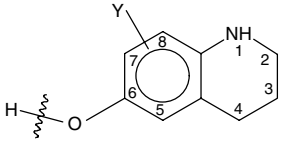
Y = 2,2,6,7-tetramethyl	78.8	329.7	Correlation	2000DEN/DEN
2,4,6,7-tetramethyl	78.0	326.4		
2,4,6,7-tetramethyl-2-C(O)OH	79.8	334.0		
2,2,4,6,7-pentamethyl	77.9	326.0		

2,3-dihydrobenzo(b) furan-5-ol and its 1-thio, 1-seleno, and 1-telluro analogues



X = O	81.3	340	Electrochem.	2001MAL/JON
S	80.5	337		
Se	80.5	336		
Te	80.5	337		

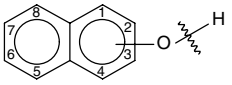
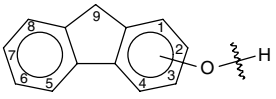
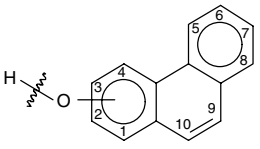
tetrahydroquinoline, substituted



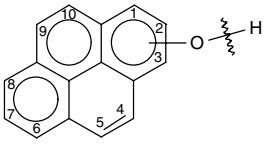
Y = 5,7,8-trimethyl-N-acetyl	83.7	350.3	Correlation	2000DEN/DEN
5,7,8-trimethyl-N-ethyl	79.6	332.9		

(continued)

Table 6.1.3 (continued) O–H BDEs in Phenols

The broken bonds (**boldface =** dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
hydroxynaphthalene, substituted 				
H–O bond at 1 site	(1) **84.5**	**353.5**	(1) Electrochem.	(1) 1975MAH/DAR
$\Delta_f H^o(R)$ = 39.5 (165.3)	(2) 84.0	351.5	(2) AOP	(2) 1991BOR/CHE(b)
	(3) 82.1	343.4	(3) Correlation	(3) 2000DEN/DEN
2 site	(1) **86.5**	**361.9**		
$\Delta_f H^o(R)$ = 41.6 (174.1)	(2) 88.0	368.2		
	(3) 84.6	353.8		
1 site with 5-OH	(1) 83.6	349.8		
2 site with 6-Br	(2) 88.5	370.3		
hydroxyfluorene 				
H–O bond at 1 site	(1) 82.0	343.1	(1) Electrochem.	(1) 1975MAH/DAR
3 site	(2) 80.9	338.3	(2) Correlation	(2) 2000DEN/DEN
hydroxy-phenanthrene 				
H–O bond at 1 site	84.8	354.7	Correlation	2000DEN/DEN
2 site	87.7	367.0		
3 site	86.6	362.5		
4 site	85.1	356.2		

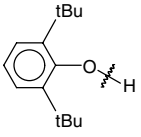
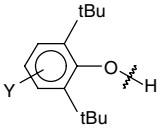
pyrene, substituted



H–O bond at 3 site		(1) 80.2	335.6	(1) Electrochem.	(1) 1975MAH/DAR
	3 site with 8-OH	(1) 79.0 (2) 75.5	330.5 315.9	(2) Correlation	(2) 2000DEN/DEN
	3 site with 10-OH	(1) 79.2 (2) 75.9	331.4 317.7		

6.1.4 O–H bonds in sterically hindered phenols

Table 6.1.4 O–H BDEs in Sterically Hindered Phenols

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
phenols, substituted  	(2) 82.1 (4) 82.8±0.2 (8) 82.7 (13) 85.1 (14) 82.8	343.5 346.4±0.8 346.0 356.1 346.4	(2) AOP (4) EPR (8) AOP (13) Electrochem. (14) Correlation	(2) 1991BOR/CHE(b) (4) 1996LUC/PED (8) 1997ZHU/ZHA (13) 1975MAH/DAR (14) 2000DEN/DEN
phenols, substituted  				
Y = p-Cl	(14) 82.3 (15) 82.4	344.5 344.8	(2) AOP	(2) 1991BOR/CHE(b)
p-NC	(14) 84.2	352.4	(4) EPR	(4) 1996LUC/PED
p-HS	(14) 81.3	340.0	(6) EPR	(6) 1973MAN/MEN

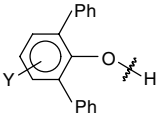
(continued)

Table 6.1.4 (continued) O–H BDEs in Sterically Hindered Phenols

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
p-Me	(4) 81.0 (7) 80.5±0.9 (8) 80.1 (17) 79.9±0.2 (18) 79.9±0.1	338.9 336.9±3.6 335 334.3±0.8 334.4±0.5	(7) EPR	(7) 2001SIL/MAT
p-Et	(8) 80.1	335.0	(8) AOP	(8) 1997ZHU/ZHA
p-NO	(14) 82.7	346.0	(9) AOP	(9) 1994ZHA/BOR
p-NO_2	(8) 86.3 (10) 86.7 (14) 85.6 (15) 84.9	361.0 362.8 358.0 355.2	(10) Electrochem.	(10) 1991PAR/HAN
p-NH_2	(14) 80.0	334.6	(11) EPR	(11) 1994LUC/PED
p-NH_2CH_2	(14) 77.2	322.9	(14) Correlation	(14) 2000DEN/DEN
p-CN	(15) 84.2	352.4	(15) EPR	(15) 2002BRI/LUC
p-MeO	(4) 78.3 (8) 79.6 (9) 79.7 (11) 77.6±0.4 (14) 78.2	327.6 333.0 333.5 324.7±1.3 327.1	(16) EPR	(16) 1994LUC/PED
p-MeC(O)NH	(14) 78.1	326.7	(17) EPR	(17) 1988COR/COL
p-$HO(O)CCH_2$	(14) 80.5	336.9	(18) EPR	(18) 2000PED/COR
p-$MeC(O)CH_2$	(14) 81.9	342.8		
p-$CNCH_2$	(14) 74.4	311.1		
p-MeC(O)	(14) 83.1	347.8		
p-HC(O)	(14) 83.1 (15) 84.2	347.8 352.3		
p-HO(O)C	(14) 83.4 (15) 84.3	348.8 352.7		
p-MeOC(O)	(8) 82.7 (9) 84.3 (15) 84.1	346.0 352.7 351.9		

p-tBuOC(O)	(14) 83.1	347.8		
p-tBu	(6) 81.2	339.7		
	(8) 82.2	344.0		
	(9) 82.6	345.6		
	(11) 81.2±0.1	339.7±0.4		
	(18) 81.3	334.0		
p-tBuO	(14) 79.2	331.3		
p-BuS	(14) 81.5	341.0		
p-RS	(16) 81.0	338.9		
p-Ph	(14) 80.7	337.7		
	(15) 81.2	339.7		
p-PhO	(14) 80.6	337.2		
p-PhS	(14) 82.8	346.4		
p-$PhCH_2$	(14) 81.2	339.7		
p-PhCH=CH	(15) 78.9	330.1		
p-Ph_2CH	(14) 81.8	342.3		
p-$(CH_2)_2Ph$	(14) 81.3	340.0		
p-$(CH_2)_2tBu$	(14) 81.2	339.8		
p-$C_{18}H_{37}OC(O)CH_2CH_2$ (octadecyloxyoxo-2′-ethyl)	(14) 81.2	339.8		
p-$C_{18}H_{37}O$ (octadecyloxy)	(14) 78.5	328.6		
p-$C_{24}H_{49}O$ (tetracozyloxy)	(14) 78.7	329.2		

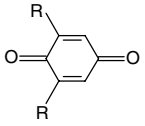
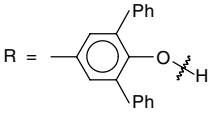
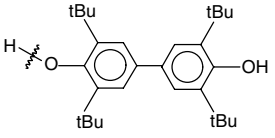
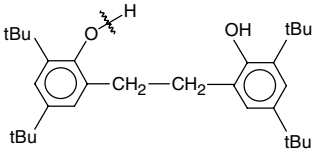
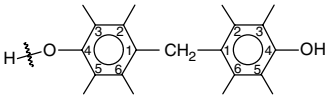
phenols, substituted

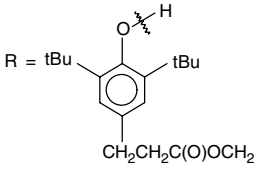
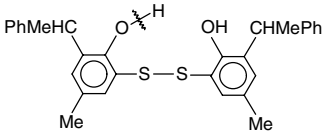
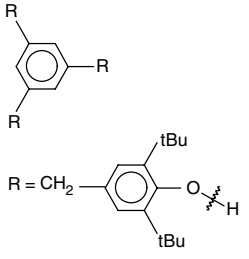
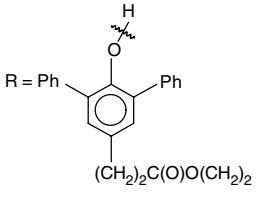
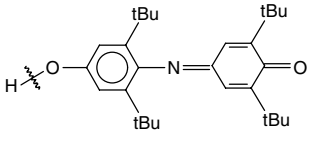


Y = Ph	(8) 84.8	355.0	(8) AOP	(8) 1997ZHU/ZHA
	(9) 85.3	356.9	(9) AOP	(9) 1994ZHA/BOR
$HO(O)CCH_2$	(14) 77.9	325.9	(14) Correlation	(14) 2000DEN/DEN

(continued)

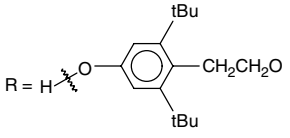
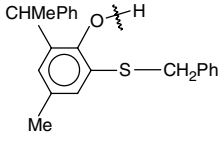
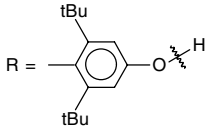
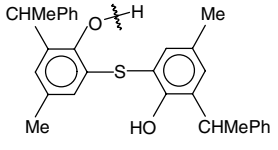
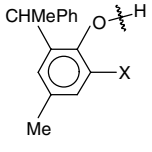
Table 6.1.4 (continued) O–H BDEs in Sterically Hindered Phenols

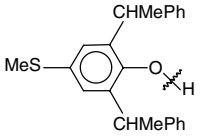
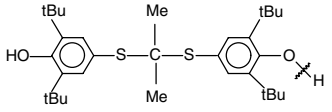
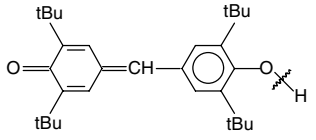
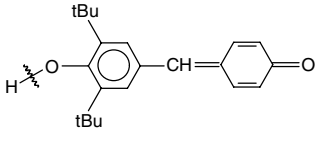
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
phenols, substituted O–H bond  	81.3	340.0	Correlation	2000DEN/DEN
phenols, substituted 	81.9	342.8	Correlation	2000DEN/DEN
ethane, substituted O–H bond 	81.5	341.0	Correlation	2000DEN/DEN
methane, substituted O–H bond 				
3,5-Bu_2	81.3	340.0	Correlation	2000DEN/DEN
2,6-Bu_2	81.4	340.5		

methane, substituted O–H bond, CR_4 	81.5	340.9	Correlation	2000DEN/DEN
disulfide, substituted O–H bond 	80.0	334.8	Correlation	2000DEN/DEN
benzene, substituted O–H bond 	82.4	344.9	Correlation	2000DEN/DEN
ether, substituted O–H bond, R–O–R 	81.0	339.0	Correlation	2000DEN/DEN
indophenol, substituted 	78.2	327.1	Correlation	2000DEN/DEN

(continued)

Table 6.1.4 (continued) O–H BDEs in Sterically Hindered Phenols

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
silane, substituted O–H bond, SiR_4 	81.5	341.0	Correlation	2000DEN/DEN
sulfide, substituted 	81.3	340.1	Correlation	2000DEN/DEN
sulfide, substituted O–H bond, RCH_2SCH_2R 	81.2	339.8	Correlation	2000DEN/DEN
sulfide, substituted 	80.1	335.2	Correlation	2000DEN/DEN
sulfide, substituted 				

X = $S(CH_2)_4CN$	82.6	345.5	Correlation	2000DEN/DEN
SCH_2CH_3	81.4	340.7		
sulfide, substituted	81.4	340.4	Correlation	2000DEN/DEN
				
4-[(4-hydroxyphenylthio)-methylthio]phenyl, substituted	81.0±0.4	338.9±1.3	EPR	1994LUC/PED
				
4-[(4-hydrophenyl)-methylene]cyclohexa-2, 5-dien-1-one, substituted	78.8±0.3	329.7±12.6	EPR	1994LUC/PED
				
galvinol	78.7	329.1	Correlation	2000DEN/DEN
				

6.2 O–O bonds

Table 6.2 O–O BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
hydroperoxide **HO**–OH	51±1	213.4±4.2	Review	1982MCM/GOL
fluoride hydroperoxide **HO**–OF	46.1±2	192.9±8.4	Derived from $\Delta_f H^o$ in ref.	1998COL/GRE
bromine hydroperoxide **HO**–OBr	33.6±2	140.6±8.4	Derived from $\Delta_f H^o$ in ref.	1998COL/GRE
difluoroperoxide **FO**–OF	47.7	199.6	Derived from $\Delta_f H^o$ in ref.	1994FRE/KAB
dichloroperoxide **ClO**–OCl	17.9±4	74.9	Derived from $\Delta_f H^o$ in ref.	1994NIC/FRI
pernitric acid **HO**–ONO_2	39±2	163.2±8.4	Derived	1978BAL/GOL
methyl hydroperoxide **HO**–OCH_3	46.7±1.5	195.4±6.3	Derived from $\Delta_f H^o$ in ref.	2001DOR/NOV
trifluoromethyl hydroperoxide **HO**–OCF_3	48.6±5	203.3±20.9	Derived from $\Delta_f H^o$ in ref.	1997JPL
tert-butyl hydroperoxide **HO**–OtC_4H_9	43.0±0.5	179.9±2.1	Pyrolysis	1992SAH/RIG

1-hydroperoxy-2, 2-dimethylpropane **HO**–$OCH_2C(CH_3)_3$	46.3±1.9	193.7±7.9	Pyrolysis	1974BAT/CHR
methaneperoxycarboxylic acid **HO**–$OC(O)CH_3$	40.6±0.5	169.9±2.1	Pyrolysis	1992SAH/RIG
ethaneperoxycarboxylic acid **HO**–$OC(O)C_2H_5$	40.6±0.5	169.9±2.1	Pyrolysis	1992SAH/RIG
dimethyl peroxide **CH_3O**–OCH_3	37.6±2	157.3±8.4	Pyrolysis	1974BAT/CHR
ditrifluoromethyl peroxide **CF_3O**–OCF_3	(1) 46.2±1 (2) **47.5±0.5**	193.3±4.2 **198.7±2.1**	(1) Pyrolysis (2) VLPP	(1) 1976DES/FOR (2) 2000REI/PRA
diethyl peroxide **C_2H_5O**–OC_2H_5	37.9±1	158.6±4.2	Pyrolysis	1974BAT/CHR
dipropyl peroxide **nC_3H_7O**–OnC_3H_7	37.1±1	155.2±4.2	Pyrolysis	1974BAT/CHR
diiso-propyl peroxide **iC_3H_7O**–OiC_3H_7	37.7	157.7	Pyrolysis	1974BAT/CHR
disec-butyl peroxide **sC_4H_9O**–OsC_4H_9	36.4±1	152.3±4.2	Pyrolysis	1983BAT
ditert-butyl peroxide **tBuO**–OtBu	(1) 38.0±1 (2) **38.2±0.5** (3) 38.9±0.5 (4) 37.5±2.4	159.0±4.2 **159.8±2.1** 162.8±2.1 156.7±9.9	(1) Pyrolysis (2) Pyrolysis (3) VLPP (4) PAC	(1) 1983BAT (2) 1992SAH/RIG (3) 2000REI/PRA (4) 2001SAN/MUR

(continued)

Table 6.2 (continued) O–O BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
dineopentyl peroxide **tBuCH$_2$O**–OCH$_2$tBu	36.4±1	152.3	Pyrolysis	1977TRE/WRI
di-1,1-dimethylpropyl peroxide **EtC(Me)$_2$O**–OC(Me)$_2$Et	39.3±1	164.4±4.2	VLPP	1973PER/GOL
ditert-nonafluorobutyl peroxide **(CF$_3$)$_3$CO**–OC(CF$_3$)$_3$	35.5±1.1	148.5±4.6	Pyrolysis	1977IRE/GOR
di(sulfur pentafluoro) peroxide **SF$_5$O**–OSF$_5$	37.2	155.6	Pyrolysis	1978CZA/SCH
di(sulfur pentafluoro) trioxide **SF$_5$O**–OOSF$_5$	30.3	126.8	Pyrolysis	1981CZA/SCH
tert-butyl 1,1-dimethyl-1-silaethyl peroxide **(CH$_3$)$_3$CO**–OSi(CH$_3$)$_3$	47	196.6	Pyrolysis	1978MAR/COM
2,2-diethyl-2-germabutyl tert-butyl peroxide **tBuO**–OGeEt$_3$	46	192.5	Pyrolysis	1965SKI
2,2-diethyl-2-stannabutyl tert-butyl peroxide **tBuO**–OSnEt$_3$	46	192.5	Pyrolysis	1961HER

trifluoromethoxy-trifluoro-methyl peroxide **CF_3OO**–OCF_3	30.3±2	126.8±8.4	Pyrolysis	1981CZA/SCH
chlorofluorotrioxide FClOO–**O**	58.4	244.3	Review	1970ONE/BEN
chlorotrioxide ClO–**OO**	7.7	32.2	Derived from Δ_fH^o in ref.	1997JPL
diacetyl peroxide **$CH_3C(O)O$**–$OC(O)CH_3$	(1) 30.4±2 (2) 36	127.2±8.4 150.6	(1) Photodetach. (2) Derived	(1) 1975REE/BRA (2) 1998COL/GRE
propanoyloxy propanoate **$C_2H_5C(O)O$**–$OC(O)C_2H_5$	(1) 30.4±2 (2) 36	127.2±8.4 150.6	(1) Photodetach. (2) Derived	(1) 1975REE/BRA (2) 1998COL/GRE
butanoyloxy butanoate **$nC_3H_7C(O)O$**–$OC(O)nC_3H_7$	(1) 30.4±2 (2) 36	127.2±8.4 150.6	(1) Photodetach. (2) Derived	(1) 1975REE/BRA (2) 1998COL/GRE

6.3 O–C bonds

6.3.1 O–C bonds in alcohols

Table 6.3.1 O–C BDEs in Alcohols

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
trifluoromethanol **HO**–CF_3	≤115.2±0.3	≤482.0±1.3	PIMS	1997ASH/APP
methanol **HO**–CH_3	(1) 92.7±0.2	387.9±0.8	(1) Derived from Δ_fH^o in ref.	(1) 1986PED/NAY
	(2) 92.8	388.3	(2) Derived	(2) 2001KOS/MIR(a)
	(3) **92.00±0.17**	**384.93±0.71**	(3) Recommend.	(3) 2002RUS/WAG

(continued)

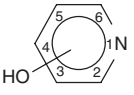
Table 6.3.1 (continued) O–C BDEs in Alcohols

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
ethanol **HO**–C_2H_5	94.0±0.7	393.3±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2,2-trifluoroethanol **HO**–CH_2CF_3	98.1±2	410.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
allyl alcohol **HO**–$CH_2CH{=}CH_2$	80.0±1	334.7±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-propen-1-ol **HO**–$CH{=}CHCH_3$	103.0±1.5	431.0±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
1-propanol **HO**–nC_3H_7	94.2±0.7	394.1±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-propanol **HO**–iC_3H_7	95.6±1	400.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-butanol **HO**–nC_4H_9	93.7±1	392.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-butanol **HO**–sC_4H_9	95.2±1	398.3±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-1-propanol **HO**–iC_4H_9	94.7±1	396.2±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-2-propanol **HO**–tC_4H_9	95.7±1	400.4±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

1-pentanol **HO**–nC_5H_{11}	92.8±1.5	388.3±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-pentanol **HO**–$CH(CH_3)(nC_3H_7)$	95.7±1	400.4±4.2	Derived from $\Delta_f H^o$ in ref.	2002CRC
3-pentanol **HO**–$CH(C_2H_5)_2$	95.9±1	401.2±4.2	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-methyl-2-butanol **HO**–$C(CH_3)_2(C_2H_5)$	95.1±1.5	397.9±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
1-hexanol **HO**–C_6H_{13}	92.9±2	388.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-hexanol **HO**–C_6H_{13}	96.1±1.5	402.1±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
phenol **HO**–C_6H_5	111.3±1	465.7±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pentafluorophenol **HO**–C_6F_5	107	447.7	Derived	1975CHO/GOL
benzyl alcohol **HO**–$CH_2C_6H_5$	(1) 81.2 (2) **81.8±1.8**	339.7 **342.3±7.5**	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1979ROS/GOL (2) 1986PED/NAY
cyclopentanol c-C_5H_9–**OH**	92.7±1.5	387.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclohexanol c-C_6H_{11}–**OH**	95.8±1.5	400.8±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 6.3.1 (continued) O–C BDEs in Alcohols

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
1-adamantanol 1-adamantyl-**OH**	(1) 92.5	387.9	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1988LIA/BAR
	(2) 91.6	383.3	(2) Derived	(2) 2001MAT/LEB
2-adamantanol 2-adamantyl-**OH**	98.5	412.1	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
1-naphthol 1-$C_{10}H_7$–**OH**	112.5±1.5	470.7±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-naphthol 2-$C_{10}H_7$–**OH**	112.3±1.5	469.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dimethylaminomethanol $(CH_3)_2(NH_2)C$–**OH**	74.7±1.5	312.5±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
pyridinol, **HO**-pyridinyl  				
2-OH	95.9±1	401.2±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
3-OH	113.3±2	474.0±8.4		
4-OH	112.7±2	471.5±8.4		

6.3.2 O–C bonds in ethers

Table 6.3.2 O–C BDEs in Ethers

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
dimethyl ether **CH_3**–OCH_3	83.2±1.0	348.1±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl methyl ether **CH_3**–OC_2H_5	83.1±1.0	347.7±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl methyl ether CH_3O–**C_2H_5**	84.2±1.3	352.3±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
divinyl ether **C_2H_3**–OC_2H_3	78.0±2.5	326.4±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
ethyl vinyl ether **C_2H_3**–OC_2H_5	101.6±1.5	425.1±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl vinyl ether **C_2H_5**–OC_2H_3	65.2±2.5	272.8±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-chloroethyl vinyl ether **CH_2ClCH_2**–OC_2H_3	66.0±2.5	276.1±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
diethyl ether **C_2H_5**–OC_2H_5	84.9±1.5	355.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-chloroethyl ethyl ether **CH_2ClCH_2**–OC_2H_5	90.5±2	379.1±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC

(continued)

Table 6.3.2 (continued) O–C BDEs in Ethers

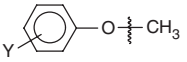
The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
methyl 2-methyl-vinyl ether **CH_3**–OC(CH_3)=CH_2	66.3	277.4	VLPP	1978ZAB/BEN
methyl propyl ether **CH_3**–OnC_3H_7	84.8±1.5	354.8±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
methyl propyl ether **CH_3O–nC_3H_7**	84.8±1.5	354.8±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
iso-propyl methyl ether **CH_3**–OiC_3H_7	82.8±1.5	346.4±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
iso-propyl methyl ether **CH_3O–iC_3H_7**	85.3±1.0	356.9±4.2	Derived from $\Delta_f H^o$ in ref.	2002CRC
ethyl propyl ether **C_2H_5**–OC_3H_7	84.8±2.0	354.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl propyl ether **C_2H_5O–C_3H_7**	84.8±1.2	354.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propyl vinyl ether **C_2H_3**–OC_3H_7	103.0±2.2	431.0±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propyl vinyl ether **C_3H_7**–OC_2H_3	65.5±2.5	274.1±10.5	Derived from $\Delta_f H^o$ in ref.	1994PED
butyl methyl ether **C_4H_9**–OCH_3	81.8±1.5	342.3±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC

butyl methyl ether $\mathbf{C_4H_9}O\mathbf{-CH_3}$	84.4±1.5	353.1±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
tert-butyl methyl ether $\mathbf{tC_4H_9}\mathbf{-}OCH_3$	83.5±1.5	349.4±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl methyl ether $\mathbf{tC_4H_9}O\mathbf{-CH_3}$	80.6±1.5	337.2±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
ethyl propyl ether $\mathbf{C_2H_5}\mathbf{-}OC_3H_7$	86.3±2.2	361.1±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl propyl ether $\mathbf{C_2H_5}O\mathbf{-C_3H_7}$	85.2±1.5	356.5±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butyl vinyl ether $C_4H_9O\mathbf{-C_2H_3}$	100.2±2.0	419.2±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butyl vinyl ether $\mathbf{C_4H_9}\mathbf{-}OC_2H_3$	65.3±2.5	273.2±10.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
tert-butyl ethyl ether $\mathbf{tC_4H_9}\mathbf{-}OC_2H_5$	82.9±1.5	346.9±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
tert-butyl ethyl ether $tC_4H_9O\mathbf{-C_2H_5}$	81.1±1.5	339.3±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
dipropyl ether $\mathbf{C_3H_7}\mathbf{-}OC_3H_7$	86.5±2.2	361.9±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
diiso-propyl ether $\mathbf{iC_3H_7}\mathbf{-}OiC_3H_7$	84.8±2.0	354.8±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 6.3.2 (continued) O–C BDEs in Ethers

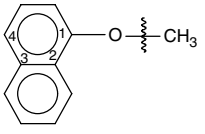
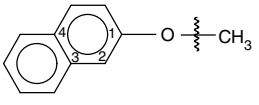
The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-ethyl-2-methylpropane **$(C_2H_5)C(CH_3)_2$**–OCH_3	84.4±2.0	353.1±8.4	Derived from Δ_fH^o in ref.	1994PED
tert-butyl isopropyl ether **tC_4H_9**–OiC_3H_7	84.7±2.0	354.4±8.4	Derived from Δ_fH^o in ref.	1994PED
tert-butyl isopropyl ether tC_4H_9O–**iC_3H_7**	84.3±2.0	352.7±8.4	Derived from Δ_fH^o in ref.	1994PED
dibutyl ether **nC_4H_9**–OnC_4H_9	83.3±2.0	348.5±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
disec-butyl ether **sC_4H_9**–OsC_4H_9	85.9±2.0	359.4±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
ditert-butyl ether **tC_4H_9**–OtC_4H_9	75.8±2.0	317.1±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
butyl tert-butyl ether **nC_4H_9**–OtC_4H_9	82.3±2.0	344.3±8.4	Derived from Δ_fH^o in ref.	1994PED
butyl tert-butyl ether nC_4H_9O–**tC_4H_9**	83.2±2.0	348.1±8.4	Derived from Δ_fH^o in ref.	1994PED
sec-butyl tert-butyl ether **tC_4H_9**–OsC_4H_9	85.8±2.0	359.0±8.4	Derived from Δ_fH^o in ref.	1994PED
sec-butyl tert-butyl ether tC_4H_9O–**sC_4H_9**	84.7±2.0	354.4±8.4	Derived from Δ_fH^o in ref.	1994PED

iso-butyl tert-butyl ether **iC$_4$H$_9$**–OtC$_4$H$_9$	82.6±2.0	345.6±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
pentyl tert-butyl ether **nC$_5$H$_{11}$**–OtC$_4$H$_9$	81.7±2.0	341.8±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
methoxybenzene or anisole **C$_6$H$_5$**–OCH$_3$	99.2±1.4	415.1±5.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methoxybenzene or anisole **CH$_3$**–OC$_6$H$_5$	(1) 64.8 (2) 65.2 (3) 65.3 (4) **64.2±1.7**	271.1 272.8 273.2 **268.6±7.1**	(1) VLPP (2) Tubular flow reactor (3) VLPP (4) Derived from $\Delta_f H^o$ in ref.	(1) 1989SUR/KAF (2) 1993ARE/LOU (3) 2001PRA/HEE (4) 1986PED/NAY
methyl pentafluorophenyl ether **CH$_3$**–OC$_6$F$_5$	60.8	254.4	VLPP	1989SUR/KAF
anisoles, substituted  Y				
Y = m-F	(1) 64.4	269.4	VLPP	(1) 1989SUR/KAF(b)
o-F	(1) 61.6	257.7		(2) 1989SUR/KAF
p-F	(1) 62.4	261.1		(3) 2001PRA/HEE
m-Cl	(2) 63.7	266.5		
o-Cl	(2) 61.3	256.5		
p-Cl	(2) 62.4	261.1		
o-Br	(2) 61.8	258.6		
m-NH$_2$	(1) 63.1	264.0		
o-NH$_2$	(1) 56.1	234.7		
p-NH$_2$	(1) 60.5	253.1		
m-OH	(2) 63.8	266.9		
o-OH	(2) 56.3	235.6		

(continued)

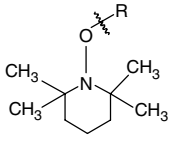
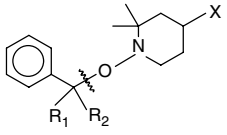
Table 6.3.2 (continued) O–C BDEs in Ethers

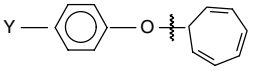
The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
	(3) 58.1	243.1		
p-OH	(2) 61.0	255.2		
	(3) 62.6	261.9		
m-Me	(1) 63.0	263.6		
o-Me	(1) 60.9	254.8		
p-Me	(1) 61.6	257.7		
m-MeO	(2) 62.4	261.1		
o-MeO	(2) 59.3	248.1		
	(3) 61.2	256.1		
p-MeO	(2) 59.3	248.1		
	(3) 62.2	260.2		
o-CH_2OH	(1) 61.0	255.2		
m-$COCH_3$	(1) 63.7	266.5		
o-$COCH_3$	(1) 62.0	259.4		
p-$COCH_3$	(1) 64.1	268.2		
o-$CH{=}CH_2$	(1) 61.0	255.2		
m-CN	(1) 64.6	270.3		
o-CN	(1) 63.4	265.3		
p-CN	(1) 63.8	266.9		
m-NO_2	(1) 63.0	263.6		
o-NO_2	(1) 62.1	259.8		
p-NO_2	(1) 64.6	270.3		
p-CF_3	(3) 67.5	282.4		
2-CHO–4-OH	(3) 62.3	260.7		
1,2-dimethoxybenzene **CH_3**–OR	60.5	253.1	VLPP	1989SUR/KAF
1,4-dimethoxybenzene **CH_3**–OR	60.7	254.0	VLPP	1989SUR/KAF

ethyl phenyl ether **C_2H_5**–OC_6H_5	(1) 64.1 (2) 65.6±2.5	268.2 274.1	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1977COL/ZAB (2) 1986PED/NAY
phenyl vinyl ether **C_2H_3**–OC_6H_5	(1) 70.0 (2) **79.1±2.5** (3) 76.0	292.9 **331.0±10.5** 318.0	(1) Pyrolysis (2) Derived from $\Delta_f H^o$ in ref. (3) Pyrolysis	(1) 1993HEN (2) 1986PED/NAY (3) 1997SCH/DOR
phenyl vinyl ether C_2H_3O–**C_6H_5**	(1) **76.6±5.0** (2) 75.9	**320.5±20.9** 317.6	(1) Derived from $\Delta_f H^o$ in ref. (2) Pyrolysis	(1) 1986PED/NAY (2) 1997SCH/DOR
diphenyl ether **C_6H_5**–OC_6H_5	(1) 75.0 (2) **79.4±2** (3) 78.8	313.8 **332.2±8.4** 329.7	(1) Pyrolysis (2) Derived from $\Delta_f H^o$ in ref. (3) Pyrolysis	(1) 1993ARE (2) 1986PED/NAY (3) 1997SCH/DOR
allyl phenyl ether **CH_2=CHCH_2**–OC_6H_5	49.8±2	208.4±8.4	VLPP	1977COL/ZAB
phenyl benzyl ether **$C_6H_5CH_2$**–OC_6H_5	52.1	218.0	Pyrolysis	1993ARE
2,3-benzoanisole 	57.5	240.6	VLPP	1989SUR/KAF
3,4-benzoanisole 	61.0	255.2	VLPP	1989SUR/KAF

(continued)

Table 6.3.2 (continued) O–C BDEs in Ethers

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
piperidinol, substituted				
				
R = CH_3	(1) 47±1	196.6	(1) VLPP	(1) 1999CIR/KOR
c-C_6H_{11}	(1) 40	167.4	(1) PAC	
C_6H_7(1, 4-cyclohexadienyl)	(1) 18	75.3	(1) PAC	
C_4H_7O(α-tetrahydrofuryl)	(1) 48	200.8	(1) PAC	
$(C_2H_5)_2NCHCH_3$	(1) 38	159.0	(1) PAC	
$C_6H_5CH_2$	(2) 32	133.9	(2) PAC	(2) 1998SKE/BEL
$C_6H_5CHCH_3$	(2) 30 (3) 33 (4) 27	125.5 138.1 113.0	(3) PAC (4) PAC	(3) 1995LI/HOW (4) 1995VER/GEO
$C_6H_5C(CH_3)_2$	(2) 26 (5) 26	108.8 108.8	(5) PAC	(5) 1998KOT/MAR
(phenylmethoxy) piperidine, substituted				
				
R_1 R_2 X			Thermolysis	1998SKE/BEL
H H H	30.6	128.0		
Me H H	28.4	118.8		
Me Me H	24.6	102.9		
H H OH	31.4	131.4		

tropylium phenoxides, substituted 				
Y = H	91.6±0.3	383.3±1.3	Electrochem.	1993ARN/FLO(b)
F	91.2±0.3	381.6±1.3		
Cl	93.4±0.4	390.8±1.7		
Br	89.0±0.4	372.4±1.7		
NO_2	93.8±0.4	392.5±1.7		
CN	93.1±0.3	389.5±1.3		
MeO	86.3±0.4	361.1±1.7		

6.3.3 O–C bonds in acids, esters, and anhydrides

Table 6.3.3 O–C BDEs in Acids, Esters, and Anhydrides

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
methyl formate **CH_3**–OC(O)H	(1) 86.8	363.2	(1) Electron capture detect.	(1) 1989CHE/ALB
	(2) 84.5±2.3	353.5±9.6	(2) Derived from $\Delta_f H^o$ in ref.	(2) 1994PED
formic acid **HC(O)**–OH	109.9±0.5	459.8±2.1	Derived from $\Delta_f H^o$ in ref.	1994LIA/LIE
acetic acid **CH_3C(O)**–OH	110.3±1	461.5±4.2	Derived from $\Delta_f H^o$ in ref.	1994LIA/LIE
propenoic acid **C_2H_3C(O)**–OH	107.7±2.5	450.6±10.5	Derived from $\Delta_f H^o$ in ref.	1998NIST

(continued)

Table 6.3.3 (continued) O–C BDEs in Acids, Esters, and Anhydrides

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
propanoic acid **$C_2H_5C(O)$**–OH	110.5±2	462.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
benzoic acid **$C_6H_5C(O)$**–OH	107.5±2.5	449.8±10.5	Derived from $\Delta_f H^o$ in ref.	1994PED
methyl acetate $CH_3C(O)O$–**CH_3**	84.3±1.2	352.7±5.0	Derived from $\Delta_f H^o$ in ref.	2002CRC
methyl acetate **$CH_3C(O)$**–OCH_3	100.5±1.5	420.5±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
ethyl chloroformate **ClC(O)**–OC_2H_5	101.7±2	425.5±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
methyl acrylate **CH_2=CHC(O)**–OCH_3	98.4±2	411.7±8.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
ethyl acetate **C_2H_5–OC(O)**CH_3	84.9±1.3	355.2±5.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iso-propyl acetate **iC_3H_7**–$OC(O)CH_3$	86.5±1.5	361.9±1.5	Derived from $\Delta_f H^o$ in ref.	1994PED
butyl acetate **C_4H_9**–$OC(O)CH_3$	85.0±1.5	355.6±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
vinyl acetate **$CH_3C(O)$**–OC_2H_3	75.8±1.5	317.1±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC

propanoinc acid ethyl ester **C_2H_5**–OC(O)C_2H_5	84.6±1.5	354.0±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
butanoic acid 1-methylpropyl ester **sC_4H_9**–OC(O)C_3H_7	86.9±1.5	363.6±6.3	Derived from $\Delta_f H^o$ in ref.	1994PED
vinyl acetate **$CH_3C(O)$**–OC_2H_3	80.3±3	336.0±12.6	Derived from $\Delta_f H^o$ in ref.	1994PED
formic acid phenyl ester **HC(O)**–OC_6H_5	74.4±3	311.3±12.6	Derived from $\Delta_f H^o$ in ref.	1994PED
acetic acid phenyl ester **$CH_3C(O)$**–OC_6H_5	77.3±3	323.4±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl benzoate **$C_6H_5C(O)$**–OCH_3	(1) 100.7±3 (2) **97.9±3**	421.3±12.6 **409.6±12.6**	(1) Derived from $\Delta_f H^o$ in ref. (2) Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY (2) 2002ROU/TEM
phenyl benzoate **$C_6H_5C(O)$**–OC_6H_5	74.8±3	313.0±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dimethoxymethane **CH_3OCH_2**–OCH_3	87.4±2.0	365.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
acetic anhydride **$CH_3C(O)$**–OC(O)CH_3	(1) 83.5 (2) **84.8±1.5**	349.4 **354.8±6.3**	(1) Electron capture detect. (2) Derived from $\Delta_f H^o$ in ref.	(1) 1989CHE/ALB (2) 1986PED/NAY
propanoic anhydride **$C_2H_5C(O)$**–OC(O)C_2H_5	87.3±3	365.3±12.6	Derived from $\Delta_f H^o$ in ref.	1994PED
benzoic anhydride **$C_6H_5C(O)$**–OC(O)C_6H_5	86.6±2.5	362.3±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

6.3.4 O–C bonds in peroxides and peroxys

Table 6.3.4 O–C BDEs in Peroxides and Peroxys

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
ethyl hydroperoxide $\mathbf{C_2H_5}$–OOH	79.4±5	332.2±20.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl hydroperoxide $\mathbf{tC_4H_9}$–OOH	73.9±1	309.2±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dimethyl peroxide $\mathbf{CH_3}$–$OOCH_3$	67.3±1.5	281.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
bis(trifluoromethyl) peroxide $\mathbf{CF_3}$–$OOCF_3$	86.4±2	361.5±8.4	Pyrolysis	1983BAT/WAL
tert-butylperoxide $\mathbf{tC_4H_9}$–$OOtC_4H_9$	70.7±2	295.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl peroxy CH_3–**OO**	(1) >30.3 (2) 32.2±1.5 (3) **32.7±0.9**	>126.8 134.7±6.5 **137.0±3.8**	(1) VLPR (2) Equilibrium study (3) Reanal.	(1) 1984KON/BEN (2) 1982KHA/NIA (3) 1998KNY/SLA(b)
trifluoromethyl peroxy CF_3–**OO**	35.3	147.7	Derived from $\Delta_f H^o$ in ref.	1992LIG/COX
chlorodifluoromethyl peroxy $CClF_2$–**OO**	30.5	127.6	Derived from $\Delta_f H^o$ in ref.	1992LIG/COX

dichlorofluoromethyl peroxy CCl_2F–**OO**	29.8	124.7	Derived from $\Delta_f H^o$ in ref.	1992LIG/COX
chloromethylperoxy CH_2Cl–**OO**	29.3±2.5	122.4±10.5	Reanal.	1998KNY/SLA(b)
dichloromethylperoxy $CHCl_2$–**OO**	25.9±2.0	108.2±8.2	Reanal.	1998KNY/SLA(b)
trichloromethylperoxy CCl_3–**OO**	22.0±1.5	92.0±6.4	Reanal.	1998KNY/SLA(b)
ethylperoxy C_2H_5–**OO**	(1) 34.1±0.5 (2) 31.3±1.1 (3) 35.5±2.0	142.7±2.1 130.1±4.6 148.4±8.4	(1) PIMS (2) Review (3) Reanal.	(1) 1990WAG/SLA (2) 1997BEN/COH (3) 1998KNY/SLA(b)
2-chloroethylperoxy CH_3CHCl–**OO**	31.4±0.4	131.2±1.8	Reanal.	1998KNY/SLA(b)
2,2-dichloroethylperoxy CH_3CCl_2–**OO**	26.8±0.5	112.2±2.2	Reanal.	1998KNY/SLA(b)
iso-propylperoxy iPr–**OO**	(1) 39.7 (2) 32.2±1.3 (3) 37.1±2.3	166.1 134.7±5.4 155.4±9.6	(1) PIMS (2) Review (3) Reanal.	(1) 1985SLA/RAT (2) 1997BEN/COH (3) 1998KNY/SLA(b)
allylperoxy CH_2=$CHCH_2$–**OO**	(1) 18.2 (2) 18.4	76.1 77.0	(1) Flash photolysis (2) PIMS detect.	(1) 1982MOR/PIL (2) 1998KNY/SLA
2-chloro-2-methylethyl-peroxy $(CH_3)_2CCl$–**OO**	32.5±0.9	136.0±3.8	Reanal.	1998KNY/SLA(b)

(continued)

Table 6.3.4 (continued) O–C BDEs in Peroxides and Peroxys

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
tert-butylperoxy tBu–**OO**	(1) 30.2±1.1 (2) 36.7±1.9 (3) 36.5±1.8	126.4±4.6 153.6±7.9 152.8±7.4	(1) VLPR (2) PIMS (3) Reanal.	(1) 1983HEN/BEN (2) 1986SLA/RAT (3) 1998KNY/SLA(b)
cyclohetylperoxy c-C_6H_{11}–**OO**	24	100.4	PAC	2000KRA/CIR
cyclohexadienylperoxy c-C_6H_7–**OO**	12	50.2	PAC	2000KRA/CIR
benzylperoxy $C_6H_5CH_2$–**OO**	(1) 22.0±1.5 (2) 21.0±1	92.0±6.0 87.9±4.2	(1) Photolysis (2) Laser induced fluorescence	(1) 1993FEN/NOZ (2) 1993ELM/MIN
α-OH-methylperoxy $HOCH_2$–**OO**	16.3±0.3	68.2±1.3	Review	1997BEN/COH
α-NH_2-methylperoxy NH_2CH_2–**OO**	36.5±1.8	152.8±7.4	Reanal.	1998KNY/SLA(b)
pyrrolidin-2-yl-peroxy c-C_4H_8N–**OO**	10	41.8	PAC	2000KRA/CIR
(ethylmethylamino) methyl-peroxy $(C_2H_5)N(CH_3)CH_2$–**OO**	25	104.6	PAC	2000KRA/CIR
acetyl peroxy $CH_3C(O)$–**OO**	38.7±5	161.9±20.9	Derived from $\Delta_f H^o$ in ref.	1991BRI/CAR

tetrahydrofuran-2-yl-peroxy C_4H_7O–**OO**	32	133.9	PAC	2000KRA/CIR
dioxan-2-yl-peroxy $C_4H_7O_2$–**OO**	34	142.3	PAC	2000KRA/CIR

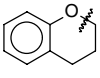
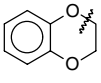
6.3.5 O–C bonds in other species

Table 6.3.5 O–C BDEs in Other Species

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
carbon dioxide **O**=CO	127.2±0.1	532.2±0.4	Spectroscopy	1970DAR
carbon oxysulfide **O**=CS	145.4	608.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
trifluoromethyl hypochlorite **ClO**–CF_3	≤88.4±0.3	≤369.9±1.3	PIMS	1997ASH/APP
methyl nitrite **Me**–ONO	58.9	246.4	Derived from $\Delta_f H^o$ in ref.	1998NIST
methyl nitrate **Me**–ONO_2	81.0	338.9	Derived from $\Delta_f H^o$ in ref.	1998NIST
1-methoxy-1,1-dimethy l-1-silaethane **Me**–$OSiMe_3$	96.3	403	Derived	1998BEC/WAL

(continued)

Table 6.3.5 (continued) O–C BDEs in Other Species

The broken bonds (**boldface** = dissociated atoms or groups)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
1-ethoxy-1,1-dimethyl-1-silaethane **Et**–$OSiMe_3$	98.5	412	Derived	1998BEC/WAL
2H-3,4-dihydropyran 	61.2	256	Derived	1997DOR/PUG
2,3-dihydro-1,4-dioxin 	60.5	253	Derived	1997DOR/PUG
chromane 	60.9	255	Derived	1997DOR/PUG
2,3-dihydro-1,4-benzodioxin 	60.2	252	Tubular flow reactor	1994SCH/ARE

6.4 O–N bonds

Table 6.4 O–N BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
dinitrogen oxide O–**N_2**	40.0	167.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
nitrogen dioxide O–**NO**	72.9	305.0	Review	1965BEN
nitrate O–**NO_2**	47.3±0.8 at 0K	197.9±3.3 at 0K	Photodissocn.	1993DAV/KIM
nitric oxide NO–**NO**	9.7±0.5	40.6±2.1	Review	1976BEN
dinitrogen trioxide O_2N–**ONO_2**	8.8	36.8	Derived from $\Delta_f H^o$ in ref.	2002CRC
nitrous acid HO–**NO**	49.4	206.7	Review	1982MCM/GOL
fluoronitrooxy FO–**NO**	34.6±7	144.8±29.3	Derived from $\Delta_f H^o$ in ref.	1997JPL
chloronitrooxy ClO–**NO**	33	138.1	Derived from $\Delta_f H^o$ in ref.	1997JPL
bromonitrooxy BrO–**NO**	16.3±2	68.2±8.4	Derived from $\Delta_f H^o$ in ref.	1998COL/GRE

(continued)

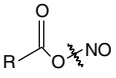
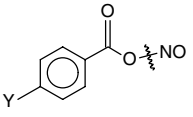
Table 6.4 (continued) O–N BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitric acid HO–**NO_2**	49.3	206.3	Derived from $\Delta_f H^o$ in ref.	1982MCM/GOL
fluoronitrooxy FO–**NO_2**	30.8±3	128.9±12.6	Derived from $\Delta_f H^o$ in ref.	1997JPL
chloronitrooxy ClO–**NO_2**	26.6±3	111.3±12.6	Derived from $\Delta_f H^o$ in ref.	1990AND/FAH
bromonitrooxy BrO–**NO_2**	27.8±3	116.3±12.6	Derived from $\Delta_f H^o$ in ref.	1996ORL/TYN
nitric peracid HOO–**NO_2**	(1) 23±2 (2) 24.1 (3) 22.8±0.8 at 0K	96.2±8.4 100.8 95.3±3.4 at 0K	(1) Pyrolysis (2) Derived from $\Delta_f H^o$ in ref. (3) Derived	(1) 1978BAL/GOL (2) 1994NIST (3) 1995ZAB
methyl nitrite CH_3O–**NO**	41.8±1	174.9±4.2	Pyrolysis	1977BAT/MIL
ethyl nitrite C_2H_5O–**NO**	42.0±1.3	175.7±5.4	Pyrolysis	1977BAT/MIL
propyl nitrite nC_3H_7O–**NO**	40.1±1.8	167.8±7.5	Pyrolysis	1974BAT/CHR
1-propyl nitrite iC_3H_7O–**NO**	41.0±1.3	171.5±7.5	Pyrolysis	1974BAT/CHR
butyl nitrite nC_4H_9O–**NO**	42.5±1.5	177.8±6.5	Pyrolysis	1974BAT/CHR

iso-butyl nitrite iC_4H_9O–**NO**	42.0±1.5	175.7±6.5	Pyrolysis	1974BAT/CHR
sec-butyl nitrite sC_4H_9O–**NO**	41.5±0.8	173.6±3.3	Pyrolysis	1974BAT/CHR
tert-butyl nitrite tC_4H_9O–**NO**	40.9±0.8	171.1±3.3	Pyrolysis	1974BAT/CHR
tert-amyl nitrite tAmO–**NO**	40.9±1	171.1±0.4	Kinetics	1979ISL
alkyl nitrite RO–**NO**	40.8±1	170.7±4.2	Review	1981BAT/ROB
phenyl nitrite C_6H_5O–**NO**	20.8	87.0	Kinetics	1998BER/CAR
alkyl nitrate RO–$\mathbf{NO_2}$	40.7±0.5	170.3±2.1	Review	1981BAT/ROB
methyl nitrate CH_3O–$\mathbf{NO_2}$	41.2±1	172.4±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl nitrate C_2H_5O–N$\mathbf{O_2}$	41.0±1	171.5±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
propyl nitrate C_3H_7O–$\mathbf{NO_2}$	42.3±1	177.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iso-propyl nitrate iC_3H_7O–$\mathbf{NO_2}$	41.1±1	172.0±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 6.4 (continued) O–N BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitrooxy acetate $CH_3C(O)OO$–**NO_2**	(1) 26.0±2 (2) **28.4±0.7**	108.8±8.4 **118.8±2.9**	(1) Pyrolysis (2) Kinetics	(1) 1977HEN/KEN (2) 1991BRI/CAR
methyl nitroperoxy CH_3OO–**NO_2**	20.7±2	86.6±8.4	Derived from $\Delta_f H^o$ in ref.	1983PAT/GOL
1-methylvinyl nitroperoxy $CH_2=C(CH_3)OO$–**NO_2**	26.0±2.0	108.8±8.4	Pyrolysis	1977HEN/KEN
(hydroxyimino)ethane **HO**–N=$CHCH_3$	49.7	207.9	Review	1970ONE/BEN
nitroso formate, substituted 				
R = CH_3	112	468.6	AOP	2000XIA/ZHU
CH_2CH_3	113	472.8		
$CH(CH_3)_2$	113	472.8		
nitroso benzoate, substituted 				
Y = H	111	464.4	AOP	2000XIA/ZHU
Br	112	468.6		
Me	110	460.2		
MeO	109	456.1		
NO_2	119	497.9		

methoxyamine CH_3O–**NH_2**	55.2	231.0	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
methylhydroxylamine **HO–**$NHCH_3$	65.4	273.6	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR

6.5 O–S, O–halogen, and O–P bonds

Table 6.5 O–S, O–Halogen, and O–P BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
oxythio radical HS–**O**	36.2	151.5	Derived from $\Delta_f H^o$ in ref.	1993BAL/CAS
sulfur dioxide **O**–SO	132±2	552.3±8.4	Spectroscopy	1970DAR
hydroxythiol **HO**–SH	70.6±4	295.4±16.7	Derived from $\Delta_f H^o$ in ref.	1993OHA/DEP
sulfur trioxide **O**–SO_2	83.2	348.1	Derived from $\Delta_f H^o$ in ref.	2002CRC
methylthio peroxy **OO**–SCH_3	11	46.0	Pulse laser photolysis	1992TUR/BAR
oxyhydrodisulfide **HO**–S_2	13.7±2	57.3±8.4	Derived from $\Delta_f H^o$ in ref.	1997JPL
sulfenic acid **HO**–SOH	75.4±3	315.5±12.6	Derived from $\Delta_f H^o$ in ref.	1978BEN

(continued)

Table 6.5 (continued) O–S, O–Halogen, and O–P BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
sulfuric acid **HO**–S(OH)O_2	(1) 93.4±2 (2) 92.5±2	390.8±8.4 387.0±8.4	Derived from $\Delta_f H^o$ in ref.	(1) 1997JPL (2) 1998CHA
methanesulfenic acid **HO**–SCH_3	73.1±3	305.9±12.6	Derived from $\Delta_f H^o$ in ref.	1996HUN/SHE
methanesulfonic acid **HO**–SO_2CH_3	86.6±3	362.3±12.6	Derived from $\Delta_f H^o$ in ref.	2000GUT/GAL
trifluoromethyl hypofluorite **F**–OCF_3	43.5±0.5	182.0±2.1	Pyrolysis	1968CZA/CAS
hydrochlorous acid **Cl**–OH	(1) 60±3 (2) 56.2 (3) **57.2**	251.0±12.6 235.1 **239.3**	(1) Review (2) Derived from $\Delta_f H^o$ in ref. (3) Derived from $\Delta_f H^o$ in ref.	(1) 1966KER (2) 1998CHA (3) 2002CRC
trifluoromethyl hypochlorite **Cl**–OCF_3	≤52.8±2	≤220.9±8.4	PIMS	1997ASH/RUS
chlorine dioxide **O**–ClO	59.0±3.0	246.9±12.6	Pyrolysis	1968CZA/CAS
bromine dioxide **O**–BrO	50.4±2.0	210.9±8.4	Derived from $\Delta_f H^o$ in ref.	2001KLE/THO
hydrobromous acid **Br**–OH	(1) 56±3 (2) 51±1	234.3±12.6 213.4±4.2	Review	(1) 1966KER (2) 1999JUR

hydroiodous acid **I**–OH	(1) 56.0±3 (2) >**50.9**	234.3±12.6 >**213.0**	(1) Review (2) Derived from $\Delta_f H^o$ in ref.	(1) 1966KER (2) 2000GIL/TAL
trifluorophosphino-1-one **O**=PF_3	(1) 130±5 (2) 129	543.9±20.9 539.8	Review	(1) 1966KER (2) 1973BEN
trichlorophosphino-1-one **O**=PCl_3	(1) 122±5 (2) 124	510.4±20.9 518.8	Review	(1) 1966KER (2) 1973BEN
tribromophosphino-1-one **O**=PBr_3	(1) 119±5 (2) 122	497.9±20.9 510.4	Review	(1) 1966KER (2) 1973BEN
triethylphosphino-1-one **O**=$P(CH_3)_3$	139	581.6	Review	1973BEN
ethyl ethylphosphate **O**=$P(OC_2H_5)_3$	148	619.2	Review	1973BEN
phosphinotris (dimethylamino)-1-one **O**=$P(N(CH_3)_2)_3$	128	535.6	Review	1973BEN
triphenylphosphino-1-one **O**=PPh_3	130	543.9	Review	1973BEN

chapter seven

Tabulated BDEs of N–X bonds

7.1 N–H bonds

7.1.1 N–H bonds in Nonanilines

Table 7.1.1 N–H BDEs in Nonanilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
ammonia **H**–NH_2 $\Delta_f H^o(R)$ = 45.1±0.3 (188.7±1.3)	(1) **108.2±0.3** (2) 107.57±0.06	**452.7±1.3** 450.08±0.24	(1) Recommended (2) Photolysis	(1) 1994BER/ELL (2) 1996MOR/ASH
difluoroammonia **H**–NF_2	75.7±2.5	316.7±10.5	Calorimetry	1969PAN/ZER
hydrazoic acid **H**–N_3 $\Delta_f H^o(R)$ = 112±5 (468.6±20.9)	(1) 92±5 (2) 94 (3) 92.7±3.1 (4) <88.7±0.5 at 0K (5) **93.8±5**	384.9±20.9 393.3 387.9±13.0 <371.1±2.1 at 0K **392.5±20.9**	(1) ICR (2) AOP (3) Correlation (4) UV photolysis (5) Derived from $\Delta_f H^o$ in ref.	(1) 1981PEL/JAC (2) 1991BOR/CHE (3) 1993JEN (4) 1999ZHA/XU (5) 2002CRC
nitrosyl hydride **H**–NO $\Delta_f H^o(R)$ = 21.58 (90.29)	46.9±0.1	196.2±0.4	Spectrometry	1996DIX

(continued)

Table 7.1.1 (continued) N–H BDEs in nonanilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitrous acid **H**–NO_2 $\Delta_f H^o$(R) = 7.91 (33.10)	78.3±0.5	327.6±2.1	Review	1982MCM/GOL
isocyanic acid **H**–NCO	(1) ≤ 109.6±0.4 at 0 K (2) 107.7	≤ 458.6 ±1.7 at 0 K 450.6	(1) Photolysis (2) Derived from $\Delta_f H^o$ in ref.	(1) 1996BRO/BER (2) 1998NIST
isothiocyanic acid **H**–NCS	≤ 97±0.2 at 0 K	≤ 405.8± 0.8 at 0 K	PIMS	1994RUS/BER(b)
methylamine $CH_3N\mathbf{H}_2$ $\Delta_f H^o$(R) = 44.0± 2 (184.1±8.4)	(1) 103±2.5 (2) 101.2±3 (3) **101.6±2**	431.0±10.5 423.4±12.6 **425.1±8.4**	(1) VLPP (2) AE (3) Review	(1) 1972GOL/SOL (2) 1973SHA/FRA (3) 1988COL
tert-butylamine tBuN$\mathbf{H}_2$ $\Delta_f H^o$(R) = 22.8±3.0 (95.4±12.6)	(1) 100 (2) 93.3±2 (2) 95± 2	418.4 390.4±8.4 397.5±8.4	(1) AOP (2) PAC	(1) 1998BOR/LIU (2) 2002LAL/ALL
benzylamine $C_6H_5CH_2N\mathbf{H}_2$ $\Delta_f H^o$(R) = 68.9±3 (288.3±12.6)	100	418.4	AOP	1998BOR/LIU
1-naphthanlenamine RN$\mathbf{H}_2$	89.6	374.7	Correlation	2000DEN/DEN
2-naphthanlenamine RN$\mathbf{H}_2$	90.7	379.5	Correlation	2000DEN/DEN

dimethylamine $(CH_3)_2N\mathbf{H}$ $\Delta_fH^o(R) = 37.8\pm2$ (158.2 ± 8.2)	(1) 95±2.5 (2) **94.6±2**	397.5±10.5 **395.8±8.4**	(1) VLPP (2) Review	(1) 1972GOL/SOL (2) 1988COL
propylamine phosphonium bromide $(n\text{-}PrN\mathbf{H}\text{–}P^+Ph_3)Br^-$	92.7	387.9	AOP	1995CHE/LIU
hydrazine $\mathbf{H}\text{–}NHNH_2$ $\Delta_fH^o(R) = 58.2$ (243.5)	87.5	366.1	Pyrolysis	1988GRE/COL
amonomethanenitrile $N\mathbf{H}_2CN$	99	414.2	AOP	1990BOR/HAR(b)
urea $(N\mathbf{H}_2)_2C{=}O$ $\Delta_fH^o(R) = 0.2\pm3.0$ (0.8 ± 12.6)	111	464.4	AOP	1991BOR/JI(b)
thiourea $(N\mathbf{H}_2)_2C{=}S$ $\Delta_fH^o(R) = 46.4\pm3$ (194.1 ± 12.6)	93	389.1	AOP	1991BOR/JI(b)
1-aminoethane-1-thione $CH_3CSN\mathbf{H}_2$	91	380.7	AOP	1991BOR/JI(b)
aminophenylmethane-1-thione $PhCSN\mathbf{H}_2$	91	380.7	AOP	1991BOR/JI(b)
bis(phenylamino)methane-1-thione $(PhN\mathbf{H})_2C{=}S$	87	364.0	AOP	1991BOR/JI(b)

(continued)

Table 7.1.1 (continued) N–H BDEs in Nonanilines

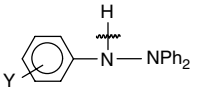
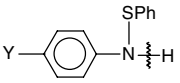
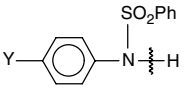
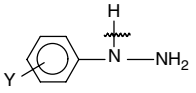
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
aminomethanamidine $(N\mathbf{H}_2)_2C{=}NH$ $\Delta_f H^o(R) = 59.9\pm3$ (250.6±12.6)	104	435.1	AOP	1991BOR/JI(b)
diphenylmethanimine $Ph_2C{=}N\mathbf{H}$	117	489.5	AOP	1991BOR/JI(b)
benzylphenylthioamine $C_6H_5CH_2N\mathbf{H}SPh$	86.9	363.6	AOP	1998BOR/LIU
formamide $HCON\mathbf{H}_2$ $\Delta_f H^o(R) = 11.9\pm3$ (49.8±12.6)	108.5	454.0	AOP	1995BOR/ZHA
acetamide $CH_3CON\mathbf{H}_2$ $\Delta_f H^o(R) = -1.6\pm3$ (–6.7±12.6)	107.5	449.8	AOP	1991BOR/JI(b)
2-ethyl-pentanamide $Et_3CCON\mathbf{H}_2$	109	456.1	AOP	1995BOR/ZHA
tert-butanamide $tBuCON\mathbf{H}_2$	109	456.1	AOP	1995BOR/ZHA
benzamide $PhCON\mathbf{H}_2$	107	447.7	AOP	1991BOR/JI

methyl aminooate $CH_3OC(O)N\mathbf{H}_2$	105	439.3	AOP	1997ZHA/BOR
ethyl aminooate $C_2H_5OC(O)N\mathbf{H}_2$	105.3	440.6	AOP	1994ZHA/BOR(e)
N-methylacetamide $CH_3CON\mathbf{H}Me$	(1) 103.9 (2) **106.5**	434.7 **445.6**	AOP	(1) 1990BOR/ZHA (2) 1995BOR/ZHA
N-(tert-butyl)-2,2-dimethyl propanamine $tBuCON\mathbf{H}tBu$	110.5	462.3	AOP	1995BOR/ZHA
acetohydrazide $MeCON\mathbf{H}NH_2$	82	343.1	AOP	1997ZHA/BOR
benzenecarbohydrazide $PhCON\mathbf{H}NH_2$	80.3	336.0	AOP	1997ZHA/BOR
N-[(1E)-buta-1,3-dienyl]-benzamide $PhCON\mathbf{H}Ph$	97	405.8	AOP	1991BOR/JI(b)
benzenesulfonamide $PhSO_2N\mathbf{H}_2$	105	439.3	AOP	1997ZHA/BOR
hydrazinophenyl sulfone $PhSO_2N\mathbf{H}NH_2$	81	338.9	AOP	1997ZHA/BOR
ethanamidine $CH_3C(=NH)N\mathbf{H}_2$	102	426.8	AOP	1991BOR/JI(b)

(continued)

Table 7.1.1 (continued) N–H BDEs in Nonanilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
benzenecarboxamidine PhC(=NH)N**H**$_2$	102	426.8	AOP	1991BOR/JI(b)
diethyl(iminophenylmethyl)-amine PhC(=N**H**)NEt$_2$	119	497.9	AOP	1991BOR/JI(b)
[(1Z)-2-aza-1,2-diphenyl-vinyl]phenylamine PhC(=NPh)N**H**Ph	92	384.9	AOP	1991BOR/JI(b)
[((1Z)-2-aza-1,2-diphenyl-vinyl)amino]dimethylamine PhC(=NPh)N**H**NMe$_2$	85	355.6	AOP	1991BOR/JI(b)
[imino(phenylamino)methyl]-phenylamine (PhN**H**)$_2$C=NH	92	384.9	AOP	1991BOR/JI(b)
[(1E)-2-aza-1,2-diphenyl-vinyl(amino)amino]-dimethylamine PhC(N**H**NMe2)=NPh	84.7	354.4	AOP	1992BOR/JI
(tert-butyl)phenylthioamine tBuN**H**SPh	87.1	364.4	AOP	1998BOR/LIU
phenyl-N-(phenylcarbonyl-amino)carboxamide PhCON**H**NHCOPh	89.3	373.6	AOP	1997ZHA/BOR

diphenyl(phenylamino) amine, substituted 				
Y = H	81.1	339.3	AOP	1997ZHA/BOR
2,4-$(NO_2)_2$	83.1	347.7		
2,4,6-$(NO_2)_3$	80	334.7		
phenylphenylthioamine, substituted 				
Y = H	82.6	345.6	AOP	1998BOR/LIU
Br	83.0	347.3		
MeO	81.6	341.4		
CN	84.2	352.3		
phenyl(phenylsulfonyl)- amine, substituted 				
Y = H	93.2	389.9	AOP	1998BOR/LIU
Br	94.4	395.0		
MeO	89.1	372.8		
CN	96.6	404.2		
di-2-naphthamine $(2\text{-}C_{10}H_7)_2N\mathbf{H}$	86.1	360.2	Correlation	2000DEN/DEN
hydrazines, substituted 				

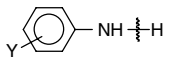
(continued)

Table 7.1.1 (continued) N–H BDEs in Nonanilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
Y = H	72.6	303.8	AOP	1997ZHA/BOR
p-Cl	73.0	305.4		
p-Me	71.9	300.8		
p-Et	76.3	319.2		
p-CF_3	77.9	325.9		
p-CN	77.8	325.5		
bis(1,1-dimethyl-1-silaethyl)-amine **H**–$N(SiMe_3)_2$	110.9	464.0	Derived	1998BEC/WAL

7.1.2 *N–H bonds in anilines*

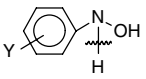
Table 7.1.2 N–H BDEs in Anilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
Aniline or benzenamine	(1) 88.0±2.0	368.2±8.4	(1) VLPP	(1) 1978COL/BEN
PhNH–**H**	(2) 92.3	386.2	(2) AOP	(2) 1993BOR/ZHA
$\Delta_f H^o(R)$ = 58.4±1	(3) 89.1	372.8	(3) Electrochem.	(3) 1994JON/LIN
(244.3±4.2)	(4) **92.2** in sol.	**385.8** in sol.	(4) PAC	(4) 1997MAC/WAY
	(4) **89.7** in gas	**375.3** in gas		
anilines, monosubstituted 				
Y = 4-F	(3) 88.8 in gas	371.5 in gas	(1) Electrochem.	(1) 1994JON/LIN
	(3) 91.3 in sol.	382.0 in sol.		
2-Cl	(4) 93.1	389.5	(2) Electrochem.	(2) 1995JON/LIN

3-Cl	(4) 92.6	387.4	(3) PAC	(3) 1997MAC/WAY
4-Cl	(4) 92.4	386.6	(4) AOP	(4) 1993BOR/ZHA
3-Br	(4) 93.2	389.9	(5) AOP	(5) 1997ZHU/ZHA
4-Br	(4) 92.3	386.2	(6) Correlation	(6) 2000DEN/DEN
4-I	(1) 89.1	372.8		
2-CN	(4) 95.1	397.9		
3-CN	(4) 94.1	393.7		
4-CN	(1) 91.8 (4) 95.2	384.1 398.3		
2-CF_3	(2) 92.5	387.0		
3-CF_3	(2) 93.2 (4) 95.7 (5) 96.6	390.0 400.4 404.2		
4-CF_3	(1) 92.0 (4) 96.5	384.9 403.8		
2-CH_3	(2) 90.6	379.0		
4-CH_3	(1) 88.7 (3) 87.5 in gas (3) 90.0 in sol. (4) 92.0	371.1 366.1 in gas 376.6 in sol. 384.9		
4-NH_2	(1) 86.0	359.8		
4-NO_2	(4) 96.7	404.6		
4-tBu	(1) 88.9 (6) 92.1	372.0 385.6		
4-CH_3CO	(1) 90.6 (3) 94.2 (4) 93.8	379.1 394.1 392.6	(1) Electrochem.	(1) 1994JON/LIN
2-CH_3O	(2) 88.7 (3) 90.4	371.0 378.2	(2) Electrochem.	(2) 1995JON/LIN
3-CH_3O	(3) 93.9	392.9	(3) AOP	(3) 1993BOR/ZHA
4-CH_3O	(1) 87.2	364.8	(4) Correlation	(4) 2000DEN/DEN
3-CF_3SO_2	(3) 95.7	400.4		
anilines, di- and trisubstituted				
2,4-Me_2	(2) 88.0	368		
3,4-Me_2	(2) 88.7	371		

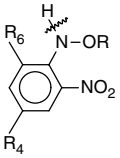
(continued)

Table 7.1.2 (continued) N–H BDEs in Anilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
3,5-Me_2	(2) 90.3	378		
2,4-$(MeO)_2$	(2) 87.7	367		
3,4-$(MeO)_2$	(2) 88.4	370		
3,5-$(MeO)_2$	(2) 91.5	383	(2) Electrochem.	(2) 1995JON/LIN
3,5$(CF_3)_2$	(4) 97.2	406.7	(4) AOP	(4) 1993BOR/ZHA
2-NO_2–4-Cl	(4) 97.6	408.4		
3-NO_2–4-Cl	(4) 97.6	408.4		
2,4,6-Cl_3	(4) 95.5	399.6		
phenylhydroxylamine 				
Y = H	69.8	292.0	AOP	1998CHE/LU
p-Me	67.9	284.1		
p-Br	72.4	302.9		
N-methyl-phenylamine PhN**H**Me $\Delta_f H^o(R)$ = 57.6±1.5 (241.0±6.3)	(1) **89.3** (2) 87.5±2 (3) 91.9	**373.6** 366.1±8.4 384.5	(1) AOP (2) VLPP (3) Correlation	(1) 1993BOR/ZHA (2) 1978COL/BEN (3) 2000DEN/DEN
phenyl-1-naphthlamine 1-$C_{10}H_7N$**H**C_6H_5	85.3	357.1	Correlation	2000DEN/DEN
phenyl-2-naphthlamine 2-$C_{10}H_7N$**H**C_6H_5	86.7	362.9	Correlation	2000DEN/DEN

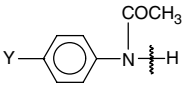
4-methoxy-N-phenyl-benzenamine 4-$CH_3OC_6H_4N\mathbf{H}Ph$	85.1	355.9	Correlation	2000DEN/DEN
N-(4-phenoxy)phenyl-2-naphthalenamine 2-$C_{10}H_7N\mathbf{H}C_6H_4$(4′-$C_6H_5O$)	83.5	349.5	Correlation	2000DEN/DEN

alkyloxy(2-nitrophenyl)amine



R	R_4	R_6				
Me	H	NO_2	75.4	315.5	AOP	1996STA/ZAR
Me	NO_2	H	76.1	318.4		
Me	NO_2	NO_2	77.6	324.7		
iPr	NO_2	NO_2	78.0	326.4		

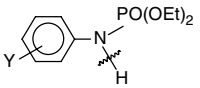
N-phenylacetamide, substituted

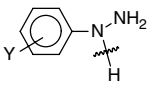
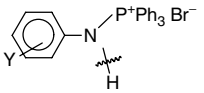


Y = H	(1) 98.9 (3) 99.5	413.8 416.3	AOP	(1) 1993BOR/ZHA(b)
p-Cl	(2) 98.7	413.0		(2) 1993CHE/ZHA
p-Br	(2) 99.1	414.6		(3) 1991BOR/JI
p-Me	(2) 97.1	406.3		
p-MeO	(2) 95.3	398.7		
p-MeCO	(2) 100.0	418.4		
p-CF_3	(2) 101.6	425.1		
p-CN	(2) 101.1 (2) 101. 5	423.0 424.7		
p-NO_2	(2) 102.0	426.8		

(continued)

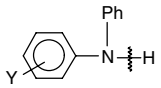
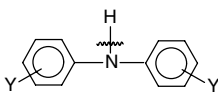
Table 7.1.2 (continued) N–H BDEs in Anilines

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
diethyl(phenylamino)-phosphino-1-one, substituted $PhN\mathbf{H}PO(OEt)_2$ 				
Y = H	(1) 94.7 (2) 94.9	396.2 397.1	AOP	(1) 1991BOR/ZHA (2) 1998CHE/LU
p-Me	(2) 93.5	391.2		
p-MeCO	(2) 97.3	407.1		
p-p-CN	(2) 98.9	413.8		
p-NO_2	(2) 100.6	420.9		
phenyl(phenylsulfonyl)amine $PhN\mathbf{H}SO_2Ph$	93.2	389.9	AOP	1998BOR/LIU
phenyl-N-benzamide $PhN\mathbf{H}COPh$	97.3	407.1	AOP	1993CHE/ZHA
(dimethylamino)-N-benzamide $PhN\mathbf{H}CONMe_2$	92.7	387.9	AOP	1998CHE/XIA
2,2,2-trifluoro-N-phenyl-acetamide $PhN\mathbf{H}COCF_3$	99.6	416.7	AOP	1993ZHA/BOR(b)
phenylphenylthioamine $PhN\mathbf{H}SPh$	82.6	345.6	AOP	1998BOR/LIU

phenyl(phenylamino)methane-1-thione PhN**H**SOPh	90.2	377.4	AOP	1998BOR/LIU
phenylhydrazine 				
X = H	72.9	305.0	AOP	1998CHE/LU
p-Me	72.2	302.1		
p-CN	77.9	325.9		
aniline phosphonium bromide, substituted 				
Y = H	68.4	286.2	AOP	1998CHE/LU
p-Me	68.8	287.9		
p-CN	64.8	271.1		
p-CF_3	64.5	269.9		
N-(phenylamino)acetamide PhNHN**H**COMe	78.6	328.9	AOP	1997ZHA/BOR
1,2-diphenylhydrazine PhN**H**NHPh	73.1	305.9	FT-ICR	1991ING/FOK
diphenylamine Ph_2N–**H** $\Delta_fH^o(R) = 87.5\pm1.5$ (366.1±6.3)	(1) 87.3 (2) 87.5 (3) 85.8±0.7 (4) 89.2 in sol. (4) **87.2** in gas (5) 87.2	365.3 366.1 359.0 373.2 in sol. **364.8** in gas 364.7	(1) Kinetics (2) AOP (3) EPR (4) PAC (5) Correlation	(1) 1987VAR/DEN (2) 1992ZHA/BOR (3) 1999LUC/PED (4) 1997MAC/WAY (5) 2000DEN/DEN

(continued)

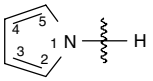
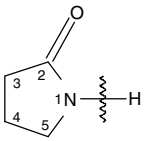
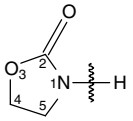
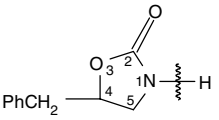
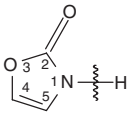
Table 7.1.2 (continued) N–H BDEs in Anilines

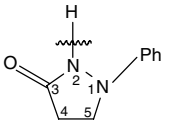
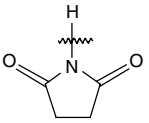
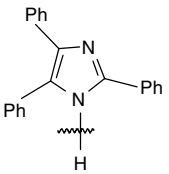
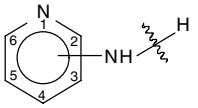
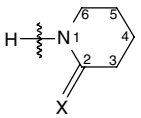
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
diphenylamine, substituted 				
Y = m-F	(1) 88.4	369.9	AOP	(1) 1993BOR/ZHA
p-Me	(1) 86.9	363.6		
m-Me	(1) 87.6	366.5		
p-MeO	(1) 85.6 (4) 85.1	358.2 356.1		
p-PhNH	(1) 79.2 (2) 79.9	331.4 334.3		(2) 1994ZHA/BOR
p-NO_2	(1) 90.4 (3) 91.0 (4) 89.1	378.2 380.7 372.9		(3) 1991BOR/ZHA (4) 2000DEN/DEN
diphenylamine, substituted 				
Y = p-Br	(1) 88.1 (2) 87.0	368.6 364.2	(1) AOP (2) Correlation	(1) 1993BOR/ZHA (2) 2000DEN/DEN
p-MeO	(1) 84.2 (2) 83.3 (4) 81.8	352.3 348.6 342.2		
p-Me	(2) 85.4 (3) 86.3 in sol. (3) **86.2** in gas (4) 83.3	357.5 361.1 in sol. **360.7** in gas 348.5	 (3) PAC (4) EPR	 (3) 1997MAC/WAY (4) 2002PRA/DIL
p-tBu	(2) 85.8	358.8		
p-$N(CH_3)_2$	(4) 79.5	332.6		
N-1-[3,7-bis(1,1-dimethyl-ethyl)naphthalenyl-benzenamine 1-(3,7-tBu_2–$C_{10}H_5$)N**H**Ph	82.4	344.9	Correlation	2000DEN/DEN

4-(1,1-dimethylethyl)-N-phenyl-benzenamine 4-tBu–$C_6H_4N\mathbf{H}Ph$	86.1	360.3	Correlation	2000DEN/DEN
N,N′-di(4-isopropylphenyl-)-p-phenylendiamine 4-tBu–C_6H_4NH–4-$C_6H_4N\mathbf{H}C_6H_4$–t-Bu	79.7	333.6	Correlation	2000DEN/DEN
N,N′-di-2-naphthyl-p-phenylendiamine 4-(2-$C_{10}H_7NH)C_6H_4N\mathbf{H}$–2′-$C_{10}H_7$	82.8	346.6	Correlation	2000DEN/DEN
N,N′-dioctyl-p-phenyl-endiamine 4-$C_8H_{17}NHC_6H_4N\mathbf{H}C_8H_{17}$	82.9	346.9	Correlation	2000DEN/DEN
N,N′-diphenyl-p-phenylen-diamine 4-C_6H_5NH–4-$C_6H_4N\mathbf{H}Ph$	85.1	355.9	Correlation	2000DEN/DEN
N-phenyl-N′-isopropyl-p-phenylendiamine 4-($C_6H_5NH)C_6H_4N\mathbf{H}$–iPr	83.5	349.2	Correlation	2000DEN/DEN
9H-carbazole 1,2-$C_6H_4N\mathbf{H}$–1′,2′-C_6H_4	88.8	371.6	Correlation	2000DEN/DEN
4-(1,1-dimethylethyl)-N-[4-(1,1-dimethylethyl)phenyl]-1-naphthalenamine 1[$N\mathbf{H}C_6H_4$–4tBu]–4′-$BuC_{10}H_6$	84.2	352.1	Correlation	2000DEN/DEN

7.1.3 N–H bonds in cyclic compounds

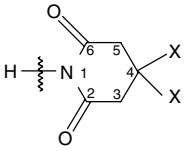
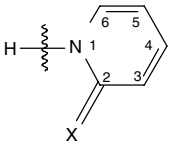
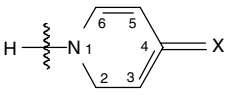
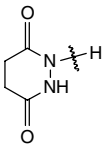
Table 7.1.3 N–H BDEs in Cyclic Compounds

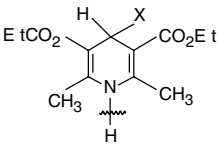
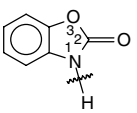
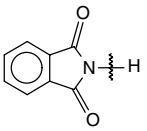
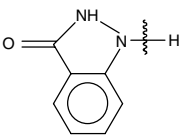
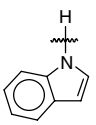
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
pyrrole 				
$\Delta_f H^o(R)$ = 70.8±3 (296.2±12.6)	(1) 99±6 (2) **97**	414.2±25.1 **405.8**	(1) Photodetach. (2) AOP	(1) 1975RIC/STE (2) 1991BOR/JI(b)
2-pyrrolidone 	107	447.7	AOP	1995BOR/SHI
1,3-oxazolidin-2-one 	105.8	442.7	AOP	1994ZHA/BOR(e)
4-benzyl-1,3-oxazolidin-2-one 	105.7	442.2	AOP	1994ZHA/BOR(e)
1,3-oxazolin-2-one 	91.0	380.7	AOP	1994ZHA/BOR(e)

1-phenylpyrazolidin-3-one 	73.9	309.2	AOP	1997ZHA/BOR
succinimide 	(1) 91.7 (2) 92.5 (3) 118±3	383.7 387.0 493.7	(1) AOP (2) AOP (3) Electrochem.	(1) 1992ARE/VEN (3) 1992BAU/DAV (3) 1993LIN/JON
2,4,5-triphenylimidazole 	89.5	374.5	AOP	1994ZHA/BOR
aminopyridine 				
H–N at site 2	87	364.0	AOP	1993BOR/SIN
3	94	393.3		
4	84	351.5		
2-piperidone, analogues 				
X = O	109.5	458.1	AOP	1995BOR/SHI
S	91	380.7		

(continued)

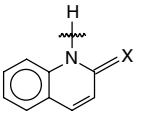
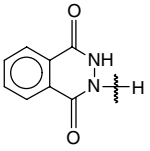
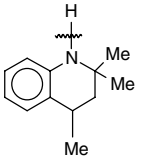
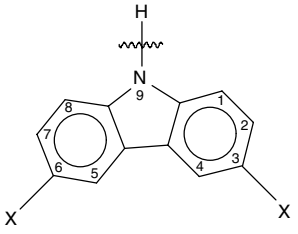
Table 7.1.3 (continued) N–H BDEs in Cyclic Compounds

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,6-piperidione 				
X = H	(1) 115±3	481.2	Electrochemical	(1) 1998LIN/MER
CH_3	(2) 104.5	437.2		(2) 1992BAU/DAV
2-pyridone, analogues 				
X = O	98	410.0	AOP	1993BOR/SIN
S	81	338.9		
4-pyridone, analogues 				
X = O	99	414.2	AOP	1993BOR/SIN
S	82	343.1		
1,2,4,5-tetrahydropyridazine-3,6-dione 	87.7	366.9	AOP	1997ZHA/BOR

1,4-dihydropyridine, substituted 				
X = H	86.2	360.7	AOP	2000CHE/LU
i-Pr	89.4	374.0		
Ph	90.8	379.9		
4-$MeOC_6H_4$	90.5	378.7		
4-MeC_6H_4	90.6	379.1		
4-ClC_6H_4	91.2	381.6		
4-CNC_6H_4	92.8	388.3		
3-hydrobenzoxazol-2-one 	94.8	396.6	AOP	1994ZHA/BOR(e)
phthalimide 	89.1	372.8	AOP	1992ARN/VEN
1H-2-hydroindazol-3-one 	77.7	325.1	AOP	1997ZHA/BOR
indole 	90.8	379.9	Electrochem.	1994JON/LIN

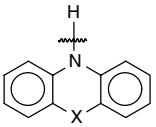
(continued)

Table 7.1.3 (continued) N–H BDEs in Cyclic Compounds

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-quinolone, analogues 				
X = O	101	422.6	AOP	1993BOR/SIN
S	83	347.3		
2,3-dihydrophthalazine-1, 4-dione 	86.8	363.2	AOP	1997ZHA/BOR
2,2,4-trimethyl-1,2,3, 4-tetrahydroquinoline 	88.1	368.6	Correlation	2000DEN/DEN
carbazole 				
X = H $\Delta_f H^o(R)$ = 91.6±2 (383.3±8.4)	(1) 92.7 (2) **93.6**	387.9 **391.6**	AOP	(1) 1991BOR/ZHA (2) 1992ARN/VEN

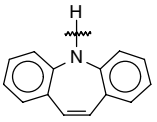
Br 3,6-dibromocarbazole	(1) 93.6 (2) 94.3	391.6 394.6		

phenothiazine, analogues

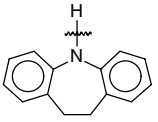


Y = O	(1) 79.7 (2) 77.2±0.3	333.5 323.0±1.3	(1) AOP (2) EPR	(1) 1993BOR/ZHA (2) 1999LUC/PED
S	(1) 82.3 (2) 79.3±0.3	344.3 331.8±1.3		
Se	(2) 80.4±0.4	336.4±1.7		

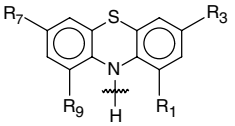
iminostilbene, or 5H-dibenzo[b,f]azepine	(1) 84.6 (2) 85.3 (3) 82.4±0.5	354.0 356.9 344.8±2.1	(1) AOP (2) AOP (3) EPR	(1) 1991BOR/CHE (2) 1994ZHA/BOR (3) 1999LUC/PED



5H,10H,11H- dibenzo[b,f]azepine	87.0	364.0	AOP	1991BOR/ZHA



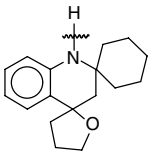
phenothioazine, substituted



$R_1 = R_9 = Me$, $R_3 = R_7 = H$	77.7±0.4	325.1±1.7	EPR	1999LUC/PED
$R_1 = R_9 = H$, $R_3 = R_7 = OMe$	76.2±0.3	318.8±1.3		
$R_1 = R_9 = H$, $R_3 = R_7 = CMe_3$	78.1±0.4	326.8±1.7		

(continued)

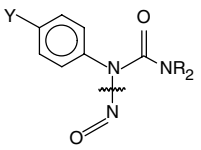
Table 7.1.3 (continued) N–H BDEs in Cyclic Compounds

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$R_1 = R_9 = H$, $R_3 = R_7 = Cl$	79.8±0.4	333.9±1.7		
$R_1 = R_9 = H$, $R_3 = R_7 = NO_2$	81.0±1.0	338.9±4.2		
2-spirocyclohexyl-4-(spiro-tetrahydrofuran-2)-1,2,3,4-tetrahydroquinoline 	86.2	360.7	Correlation	2000DEN/DEN

7.2 *N–N bonds*

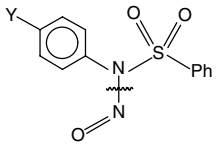
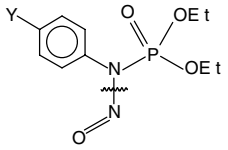
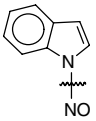
Table 7.2 N–N BDEs

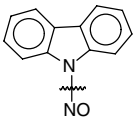
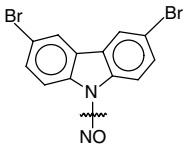
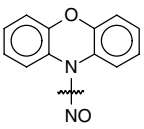
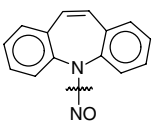
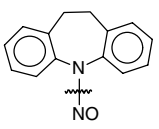
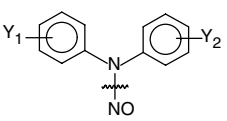
The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
dinitrogen trioxide **ON**–NO_2	8.8	36.8	Derived from $\Delta_f H^o$ in ref.	2002CRC
dinitrogen tetraoxide **O_2N**–NO_2	13.2	55.2	Derived from $\Delta_f H^o$ in ref.	2002CRC
hydrazine **H_2N**–NH_2	67.4	282.0	Derived from $\Delta_f H^o$ in ref.	2002CRC
tetrafluorohydrazine **F_2N**–NF_2	21±1	87.9±4.2	Calorimetry	1969PAN/ZER

methylhydrazine **NH_2**–$NHCH_3$	64.9±2	271.5±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,1-dimethylhydrazine **NH_2**–$N(CH_3)_2$	62.7±2	262.3±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
phenylhydrazine **NH_2**–NHC_6H_5	55.0±2	230.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1,2-dimethylhydrazine **$(CH_3)NH$**–$NH(CH_3)$	66.0±3	276.1±12.6	Derived from $\Delta_f H^o$ in ref.	2002CRC
dimethyl(methylamino)amine **$(CH_3)_2N$**–$NH(CH_3)$	60.8	254.4	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
N-nitrodimethylamine $(CH_3)_2N$–**NO_2**	(1) 43.8 (2) 39.6	183.3 165.7	(1) Derived from $\Delta_f H^o$ in ref. (2) Derived	(1) 1986PED/NAY (2) 2001KOS/MIRb
amino-N-nitroso-N-phenyl-amide, substituted  R = Me				
Y = H	92.7	387.9	AOP	1998CHE/XIA
Cl	93.4	390.8		
Br	93.5	391.2		
I	93.4	390.8		
Me	91.8	384.1		
MeO	90.4	378.2		
MeCO	94.9	397.1		
NO_2	96.4	403.3		

(continued)

Table 7.2 (continued) N–N BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitrosophenyl(phenyl-solfonyl)-amine, substituted 				
Y = H	92.6	387.4	AOP	1998CHE/XIA
Cl	93.8	392.5		
Me	91.7	383.7		
MeO	89.0	372.4		
MeCO	95.2	398.3		
NO_2	97.1	406.3		
diethyl(nitrosophenylamino)-phosphino-1-one, substituted 				
X = H	94.7	94.7	AOP	1998CHE/XIA
Cl	95.7	400.4		
Br	95.7	400.4		
Me	93.4	390.8		
NO_2	100.5	420.5		
nitrosoindole 	94.1	393.7	AOP	2000ZHU/HE

9-nitrosocarbazole 	93.0	389.1	AOP	2000ZHU/HE
3,6-dibromo-9-nitrosocarbazole 	93.8	392.5	AOP	2000ZHU/HE
10-nitrosophenoxazine 	80.0	334.7	AOP	2000ZHU/HE
5-nitroso-benzo[b,f]azepine 	84.8	354.8	AOP	2000ZHU/HE
5-nitroso-10H,11H-dibenzo[b,f]azepine 	87.2	364.8	AOP	2000ZHU/HE
nitrosodiphenylamine, substituted 				

(continued)

Table 7.2 (continued) N–N BDEs

The broken bonds (**boldface** = dissociated atom)		BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
		kcal/mol	kJ/mol		
Y_1 = H	Y_2 = H	87.7	366.9	AOP	2000ZHU/HE
m-Cl	H	88.6	370.7		
m-Me	H	87.8	367.4		
p-Me	H	87.1	364.4		
p-NO_2	H	90.6	379.1		
p-MeO	H	85.8	359.0		
p-MeO	p-MeO	84.4	353.1		
methylnitrosohydrazine $H_2NN(Me)$–**NO**		42.9	179.6	Combustion	1998LEB/CHI

7.3 N–C bonds

Table 7.3 N–C BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
diazomethane CH_2=**N_2**	< 41.8	< 174.9	UV photolysis	1971LAU/OKA
isocyanic acid **HN**=CO	≤ 122.1±0.3	≤ 510.9±1.3	Photolysis	1996BRO/BER
cyanogen azide **N_3**–CN	109.5±5	458.1±20.9	Derived from $\Delta_f H^o$ in ref.	1998NIST
1-aza-1-diazoethene **N_3**–CH_3	80.1±5	335.1±20.5	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR

azadiazophenylmethane $\mathbf{N_3}$–C_6H_5	89.8±5	374.5±20.9	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
1-aza-1-diazo-2,2,2-triphenylethane $\mathbf{N_3}$–$C(C_6H_5)_3$	46.6	195.0	Review	1974PEP/ERL
nitrosyl cyanide NC–**NO**	28.8±2.5	120.5±10.5	Electron impact	1975GOW/JON
nitrosomethane CH_3–**NO**	(1) 40.0±0.8 (2) **41.1**	167.4±3.3 **172.0**	(1) Pyrolysis (2) Visible spectroscopy	(1) 1973BAT/MIL (2) 1990MCC/PFA
nitroso-trifluoromethane CF_3–**NO**	(1) 31±3 (2) 42.8±2 (3) **39.9**	129.7±12.6 179.1±8.4 **167.0**	(1) Electron impact (2) Pyrolysis (3) Visible spectroscopy	(1) 1973CAR/GOW (2) 1979GLA/MAI (3) 1990MCC/PFA
nitroso-trichloromethane CCl_3–**NO**	(1) 32±3 (2) **29.9**	133.9±12.6 **125.0**	(1) Electron impact (2) Pulse photolysis	(1) 1973CAR/GOW (2) 1995LEY/MAS
3-nitroso-1-propene CH_2CHCH_2–**NO**	26.3	110.0	Flash photolysis	1995BOY/NOZ
2-nitroso-propane iC_3H_7–**NO**	36.5±3	152.7±12.6	Electron impact	1972CAR/GOW
nitroso-tert-butane tC_4H_9–**NO**	(1) 29±3 (2) 39.5±1.5 (3) **39.9**	121.3±12.6 165.3±6.3 **167.0**	(1) Electron impact (2) VLPP (3) Laser excitation	(1) 1973CAR/GOW (2) 1974CHO/MEN (3) 1986NOB/QUI

(continued)

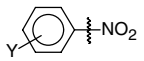
Table 7.3 (continued) N–C BDEs

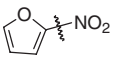
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2,2-dimethyl-1-nitrosopropane $tBuCH_2$–**NO**	36	150.6	Electron impact	1972CAR/GOW
nitrosobenzene C_6H_5–**NO**	(1) 51.5±1 (2) **54.2±0.5** (3) 52.4±1.4	215.5 **226.8±2.1** 219.2±5.9	(1) VLPP (2) Pyrolysis (3) Derived from $\Delta_f H^o$ in ref.	(1) 1975CHO/GOL (2) 1997PAR/DYA (3) 1998NIST
nitroso-pentafluorobenzene C_6F_5–**NO**	(1) 62.0±5 (2) **50.5±1**	259.4±20.9 **211.3±4.2**	(1) Electron impact (2) VLPP	(1) 1973CAR/GOW (2) 1975CHO/GOL
nitrosotoluene $C_6H_5CH_2$–**NO**	29.4	123.0	Flash photolysis	1995BOY/NOZ
nitromethane CH_3–**NO_2**	(1) **60.8** (2) 63.7 (3) 60.8	**254.4** 266.5 254.4	(1) Review (2) Electron capture detect. (3) Derived	(1) 1981BAT/ROB (2) 1989CHE/ALB (2) 2000MIR/VOR
nitroethylene C_2H_3–**NO_2**	71.5	299.2	Derived from $\Delta_f H^o$ in ref.	1999BUR
nitroethane C_2H_5–**NO_2**	(1) 58.6 (2) **60.8**	245.2 **254.4**	(1) Review (2) Derived from $\Delta_f H^o$ in ref.	(1) 1981BAT/ROB (2) 1986PED/NAY
(E)-nitro-propylene-2 $(CH_3)CH{=}CH$–**NO_2**	69.3	290.0	Derived from $\Delta_f H^o$ in ref.	1999BUR

nitrocyclopropane cyclo-C_3H_5–**NO_2**	70.6	295.4	Derived from $\Delta_f H^o$ in ref.	1999BUR
1-nitropropane nC_3H_7–**NO_2**	61.3	256.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-nitropropane iC_3H_7–**NO_2**	(1) 59.0 (2) **62.1**	246.9 **259.8**	(1) Review (2) Derived from $\Delta_f H^o$ in ref.	(1) 1981BAT/ROB (2) 1986PED/NAY
1-nitrobutane nC_4H_9–**NO_2**	(1) 60.9 (2) 61.2	254.8 256.0	Derived from $\Delta_f H^o$ in ref.	(1) 1986PED/NAY (2) 2002KOS/MIR
2-nitrobutane sC_4H_9–**NO_2**	62.9	263.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-2-nitropropane tC_4H_9–**NO_2**	(1) 58.5 (2) 61.8	244.8 258.6	(1) Review (2) Derived from $\Delta_f H^o$ in ref.	(1) 1981BAT/ROB (2) 1986PED/NAY
nitropentane nC_5H_{11}–**NO_2**	(1) 60.4±1.5 (2) 60.2±1.5	252.7±6.3 251.9±6.3	(1) Derived from $\Delta_f H^o$ in ref.	(1) 1997VER (2) 1999BUR
nitrohexane nC_6H_{13}–**NO_2**	60.2	251.9	Derived from $\Delta_f H^o$ in ref.	1999BUR
nitrobenzene C_6H_5–**NO_2**	(1) 71.3±1 (2) 71.4±2 (3) **70.7±1** (4) 71.8	298.3±4.2 298.7±8.4 **295.8±4.2** 300.4	(1) Review (2) VLPP (3) Derived from $\Delta_f H^o$ in ref. (4) Derived from $\Delta_f H^o$ in ref.	(1) 1981BAT/ROB (2) 1985GON/LAR (3) 1986PED/NAY (4) 2002KOS/MIR

(continued)

Table 7.3 (continued) N–C BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitrobenzene, substituted 				
Y = 3-NH_2 $\Delta_f H^o$(3-NH_2–C_6H_4) = 76.5 (320.1)	(1) 70.5	295.0	(1) Pyrolysis	(1) 1975MAT/NAS
Y = 4-NH_2 $\Delta_f H^o$(4-NH_2–C_6H_4) = 78.3 (327.8)	(1) 72.2	302.0		
3-NO_2 $\Delta_f H^o$(3-NO_2–C_6H_4) = 81.4±2.4 (340.6±10.0)	(1) 66.5 (2) 73.2±2.4	278.2 306.3±10.0	(2) VLPP	(2) 1985GON/LAR
4-NO_2 $\Delta_f H^o$(4-NO_2–C_6H_4) = 72.3 (302.7)	(1) 67.0	280.3		
2-Me $\Delta_f H^o$(2-Me–C_6H_4) = 75.3±2.5 (315.1±10.5)	(2) 70.2±2.5	293.7±10.5		
4-Me $\Delta_f H^o$(3-NO_2–C_6H_4) = 70.9±2.3 (296.6±9.6)	(2) 71.4±2.3	298.7±9.6		
3,5-$(NO_2)_2$ $\Delta_f H^o$(3,5-$(NO_2)_2$–C_6H_3) = 73.0 (305.4)	(1) 66.0	276.1		
2-Me-4-NO_2 $\Delta_f H^o$(2-Me-4-NO_2–C_6H_3) = 70.6±2 (295.4±8.4)	(2) 70.6±2	295.4±8.4		
phenylnitromethane $C_6H_5CH_2$–**NO_2**	49.0	205.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-nitronaphthalene 1-naphtyl-**NO_2**	77.3±1.6	323.4±6.7	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dinitromethane $R_2(NO_2)C$–**NO_2**	48.8±2.5	204.2±10.5	Review	1981BAT/ROB

dinitromethane $(NO_2)CH_2$–**NO_2**	(1) 48.8±2.5 (2) 49.5 (3) 52.2	204.2±10.5 207.1 218.4	(1) Review (2) Derived from $\Delta_f H^o$ in ref. (3) Derived	(1) 1981BAT/ROB (2) 1986PED/NAY (3) 2000MIR/VOR
trinitromethane $(NO_2)_2CH$–**NO_2**	(1) 43.7±2.5 (2) 45.1	182.8±10.5 188.9	(1) Review (2) Derived	(1) 1981BAT/ROB (2) 2000MIR/VOR
tetra-nitromethane $(NO_3)_3C$–**NO_2**	(1) 40.5±1 (2) 42.1	169.5±4.2 176.1	(1) Review (2) Derived	(1) 1981BAT/ROB (2) 2000MIR/VOR
2-nitrofuran 	70.4	294.6	Pyrolysis	1987PRO/NAZ
methylamine CH_3–**NH_2**	85.7±0.5	358.6±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
difluoro(trifluoromethyl)-amine **CF_3**–NF_2	67.7	283.3	Derived from $\Delta_f H^o$ in ref.	1977PED/RYL
ethylamine C_2H_5–**NH_2**	84.8±1.5	354.8±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclopropylamine c-C_3H_5–**NH_2**	93.4±0.6	390.8±2.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-propylamine nC_3H_7–**NH_2**	85.7±0.7	358.6±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-propylamine iC_3H_7–**NH_2**	86.1±0.9	360.2±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclobutylamine c-C_4H_7–**NH_2**	86.6±1.2	362.3±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 7.3 (continued) N–C BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
1-butylamine nC_4H_9–**NH_2**	85.7±0.7	358.2±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-butylamine sC_4H_9–**NH_2**	86.4±0.7	361.5±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iso-butylamine iC_4H_9–**NH_2**	85.4±1.2	257.3±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-2-propylamine tC_4H_9–**NH_2**	85.6±1.5	358.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclopentyamine c-C_5H_9–**NH_2**	83.5±1.2	349.4±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-pyridylamine pyridin-2-yl-**NH_2**	103.6	433.5	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
3-pyridylamine pyridin-3-yl-**NH_2**	104.6	437.6	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
4-pyridylamine pyridin-4-yl-**NH_2**	107.6	450.2	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
aniline or benzenamine C_6H_5–**NH_2**	103.2±1.0	431.8±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclohexylamine c-C_6H_{11}–**NH_2**	88.2±1.5	369.0±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

benzylamine $C_6H_5CH_2$–**NH_2**	(1) 71.1±1 (2) **72.6±1.8** (3) 72.9±1.8 (4) 72.9±1, 0 K	297.5±4.2 **303.8±7.5** 305.0±7.5 305.4	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref. (3) Derived from $\Delta_f H^o$ in ref. (4) Shock tube	(1) 1972GOL/SOL (2) 1986PED/NAY (3) 1999VER (4) 2002SON/GOL
1-naphthylamine 1-naphtyl–**NH_2**	103.4±2	432.6±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-naphthylamine 2-naphtyl–**NH_2**	108.9±2	455.6±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
formamide HC(O)–**NH_2**	101.4±2	424.3±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
acetamide $CH_3C(O)$–**NH_2**	99.7±2	417.1±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
2,2-bis(difluoroamino) propane $(CH_3)_2(NF_2)C$–**NF_2**	(1) ~47 (2) **47.8**	~196.6 **200.0**	(1) Pyrolysis (2) Pyrolysis/ FTIR	(1) 1993FOK/GRE (2) 2002PAR/CHA
methyl hydrazine CH_3–**$NHNH_2$**	70.7±2.5	295.8±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
phenyl hydrazine C_6H_5–**$NHNH_2$**	88.6±2.5	370.7±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
N,N,N′N′-methyl-methanediamine **$(CH_3)_2N$**–$CH_2N(CH_3)_2$	55.6±3	232.6±12.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dimethylamine **CH_3**–$NHCH_3$	(1) 82.2±2.5 (2) 81.9	343.9±10.5 342.7	Derived	(1) 1982MCM/GOL (2) 2001KOS/MIR(b)
ethyl methylamine **C_2H_5**–$NHCH_3$	79.8±1	333.9±4.2	Derived	1982MCM/GOL

(continued)

Table 7.3 (continued) N–C BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
phenyl methylamine **C_6H_5**–$NHCH_3$	100.6±2.5	420.9±10.5	Derived	1982MCM/GOL
benzyl methylamine **$C_6H_5CH_2$**–$NHCH_3$	68.7±2	287.4±8.4	VLPP	1972GOL/SOL
trimethylamine **CH_3**–$N(CH_3)_2$	(1) 75.5±2.5 (2) 79.3	316.3±10.5 331.8	Derived	(1) 1982MCM/GOL (2) 2001KOS/MIR(b)
ethyl dimethylamine **C_2H_5**–$N(CH_3)_2$	72.3±2	305.2±8.4	Derived	1982MCM/GOL
phenyl dimethylamine **C_6H_5**–$N(CH_3)_2$	93.2±2.5	389.9±10.5	Derived	1982MCM/GOL
benzyl dimethylamine **$C_6H_5CH_2$**–$N(CH_3)_2$	(1) 62.1±2.5 (2) 66.8	259.8±10.5 279.5	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1972GOL/SOL (2) 1999VER
1-methylpyrrile **CH_3**–pyrrol-1-yl	81.3±2	340.2±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
N-methylaniline **CH_3**–NHC_6H_5	(1) 71.4±2 (2) 68.9	298.7±8.4 288.3	(1) VLPP (2) Pyrolysis	(1) 1978COL/BEN (2) 1990BEC/DOG
N-ethylaniline **C_2H_5**–NHC_6H_5	73.3±2	306.7±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
N,N′-methylaniline **CH_3**–$N(CH_3)C_6H_5$	70.8	296.2	VLPP	1978COL/BEN

dimethyl phenylamine $C_6H_5(CH_3)N$-**CH_3**	70.8±2	296.2±8.4	VLPP	1978COL/BEN
dimethyl benzylamine $(CH_3)_2N$–**CH_2Ph**	62.1±2	259.8±8.4	VLPP	1972GOL/SOL
azomethane **CH_3**–N_2CH_3	52.5	219.7	Pyrolysis	1970BEN/ONE
azohexafluoroethane **CF_3**–N_2CF_3	55.2	231.0	Pyrolysis	1970BEN/ONE
azoethane **C_2H_5**–$N_2C_2H_5$	50	209.2	Pyrolysis	1970BEN/ONE
azoisopropane **iC_3H_7**–$N_2iC_3H_7$	47.3	197.9	Pyrolysis	1970BEN/ONE
azobutane **nC_4H_9**–$N_2nC_4H_9$	50	209.2	Pyrolysis	1970BEN/ONE
azoisobutane **iC_4H_9**–$N_2iC_4H_9$	49	205.0	Pyrolysis	1970BEN/ONE
azo-2-butane **sC_4H_9**–$N_2sC_4H_9$	46.7	195.4	Pyrolysis	1970BEN/ONE
azotertbutane **tC_4H_9**–$N_2tC_4H_9$	43.5	182.0	Pyrolysis	1970BEN/ONE
azotoluene **$C_6H_5CH_2$**–$N_2CH_2C_6H_5$	37.6	157.3	Pyrolysis	1970BEN/ONE

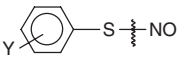
(continued)

Table 7.3 (continued) N–C BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
bis(1,1-dimethyl-silaethyl)-methylamine **CH_3**–N($SiMe_3$)$_2$	87	364	Derived	1998BEC/WAL
methyl isocyanide CH_3–**NC**	101.5±2.2	424.7±9.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl isocyanide C_2H_5–**NC**	100.1±1.7	418.8±7.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
amonomethanenitrile H_2N–**CN**	118.8±3	497.1±12.6	Derived from $\Delta_f H^o$ in ref.	2001BIS/HOO
carboxamide **HC(O)**–NH_2	99.1	414.6	Derived from $\Delta_f H^o$ in ref.	1988LIA/BAR
N,N-dimethylformamide **HC(O)**–N(CH_3)$_2$	93.7±2	392.0±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
N,N-dimethylacetamide **CH_3C(O)**–N(CH_3)$_2$	91.4	382.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
N-(aminocarbonyl)acetamide **HC(O)**–NHC(O)NH_2	115.6±2	483.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
N-methylglycine or sarcosine **HO(O)CCH_2**–$NHCH_3$	71.6±2	299.6±8.6	Derived from $\Delta_f H^o$ in ref.	2002CRC

7.4 N–S bonds

Table 7.4 N–S BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
(tert-butyl)nitrosothio t-BuS–**NO**	27.5	115.1	AOP	2001LU/WIT
(benzyl)nitrosothio $PhCH_2S$–**NO**	28.8	120.5	AOP	2001LU/WIT
(phenyl)nitrosothio, substituted 				
Y = H	19.4±1.3	81.2±5.4	AOP	2001LU/WIT
2-Cl	19.3±1.5	80.8±6.3		
3-Cl	20.9±1.4	87.4±5.9		
4-Cl	19.2±1.4	80.3±5.9		
3-Me	19.9±1.2	83.3±5.0		
4-Me	21.4±1.2	89.5±5.0		
4-MeO	21.0±1.9	87.9±7.9		
4-NO_2	18.6±1.5	77.8±6.3		

7.5 N–halogen bonds

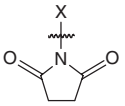
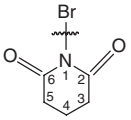
Table 7.5 N–Halogen BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitrosyl fluoride **F**–NO	56.25	235.35	Derived from $\Delta_f H^o$ in ref.	1998CHA

(continued)

Table 7.5 (continued) N–Halogen BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
nitryl fluoride **F**–NO_2	52.9	221.3	Derived from $\Delta_f H^o$ in ref.	1998CHA
nitrogen trifluoride **F**–NF_2	60.7	254.0	Derived from $\Delta_f H^o$ in ref.	1998CHA
nitrosyl chloride **Cl**–NO	38.2	159.8	Derived from $\Delta_f H^o$ in ref.	2002CRC
nitryl chloride **Cl**–NO_2	34	142.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
nitrogen chlorofluoride **Cl**–NF_2	~32	~133.9	Kinetics	1967PET
nitrosyl bromide **Br**–NO	28.7	120.1	Derived from $\Delta_f H^o$ in ref.	2002CRC
nitryl bromide **Br**–NO_2	19.6±1.7	82.0±7.1	Resonance fluorescence	1991KRE/NIC
nitrogen bromofluoride **Br**–NF_2	<54.3	<227.2	Kinetics	1972CLY/CON
nitrosyl iodide **I**–NO	18.6±0.1	77.8±0.4	UV spectrom.	1981FOR/HIP
nitryl iodide **I**–NO_2	18.3±1.0	76.6±0.4	Spectroscopy	1976VAN/TRO

N-halogenosuccinimide 				
X = Cl	(1) 73±4	305.4±16.7	Electrochem.	(1) 1993LIN/JON
Br	(2) 66±2	276.1±8.4		(2) 1998LIN/MER
1-bromo-2,6-piperidione 	65.0±2	272.0±8.4	Electrochem.	1998LIN/MER

chapter eight

Tabulated BDEs of S–X bonds

8.1 S–H bonds

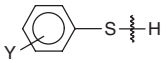
Table 8.1 S–H BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
oxythio radical **H**–SO	41.3	172.8	Kinetics	1978WHI/GAR
oxythio **H**–SOH	79.0±3.5	330.5±14.6	Ion flow tube	1993OHA/DEP
hydrogen sulfide **H**S–H $\Delta_f H^o$(R) = 34.18±0.68 (143.01±2.85)	(1) 91.1±1	381.2±4.2	(1) Iodination	(1) 1979HWA/BEN
	(2) 92.9±2	388.7±8.4	(2) Electron photodetach.	(2) 1980JAN/REE
	(3) 91.2±0.7	381.6±2.9	(3) Resonance fluorescence	(3) 1992STI/NIC
	(4) **91.2±0.7**	**381.6±2.9**	(4) Recommend.	(4) 1994BER/ELL
	(5) 91.2±0.1	381.4±0.5	(5) Photolysis	(5) 1996WIL/HOW
hydrogen disulfide **H**–SSH $\Delta_f H^o$(R) = 27.6±3.5 (115.5±14.6)	76±3.5	318.0±14.6	Ion flow tube	1993OHA/DEP
methylthiol **H**–SCH_3	(1) 88.1	369.6	(1) VLPP	(1) 1977COL/BEN(b)
	(2) 86.4±2.2	361.5±9.2	(2) Photoelectr.	(2) 1987MOR/ELL

(continued)

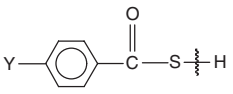
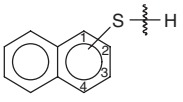
Table 8.1 (continued) S–H BDEs

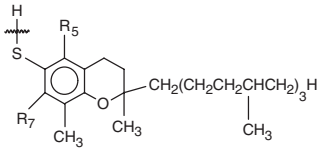
The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$\Delta_f H^o(R) = 29.8 \pm 0.4$ (124.7±1.7)	(3) 87.4	365.7	(3) Resonance fluorescence	(3) 1992NIC/KRE
	(4) **87.4±0.5**	**365.7±2.1**	(4) Recommend.	(4) 1994BER/ELL
	(5) 87.0±0.4	364.0±1.7	(5) Photolysis	(5) 1999BIS/CHO
H–SCD_3	(6) 88.3±2	369.4±8.4	(6) Electron photodetach.	(6) 1980JAN/REE
ethylthiol **H**–SC_2H_5	(1) 88.6±2	370.7±8.4	(1) Electron photodetach.	(1) 1980JAN/REE
$\Delta_f H^o(R) = 24.1$ (101)	(2) **87.3**	**365.3**	(2) Derived from $\Delta_f H^o$ in ref.	(2) 1986PED/NAY
propylthiol **H**–SC_3H_7	(1) 88.6±2	370.7±8.4	(1) Electron photodetach.	(1) 1980JAN/REE
$\Delta_f H^o(R) = 19.1$ (80)	(2) **87.4**	**365.7**	(2) Derived from $\Delta_f H^o$ in ref.	(2) 1986PED/NAY
iso-propylthiol **H**–S–iC_3H_7 $\Delta_f H^o(R) = 17.9 \pm 2$ (74.9±8.4)	88.4±2	369.9±8.4	Electron photo-detachment	1980JAN/REE
tert-butylthiol **H**–S–tC_4H_9 $\Delta_f H^o(R) = 10.5 \pm 2$ (43.9±8.4)	88.6±2	370.7±8.4	Electron photo-detachment	1980JAN/REE
alkyl thiol **H**–SR	87.4	365.7	Review	1992NIC/KRE
thioacetic acid **H**–$SCOCH_3$	88.6	370.7	Electrochem.	1999ZHA/LIN

thiobenzoic acid **H**–SCOPh	87.0	364.0	Pulse radiolysis	1998ZHA/LIN
methanedifulfide **H**–$SSCH_3$	79±3.5	330.5±14.6	Ion flow tube	1993OHA/DEP
benzenethiol PhS–**H** $\Delta_fH^o(R)$ = 58.0±1.1 (242.7±4.6)	(1) 83.3±2 (2) 79.4 (3) 80 (4) 80.8 (5) **83.5±1.1**	348.5±8.4 332.2 334.7 338.1 **349.4±4.5**	(1) VLPP (2) AOP (3) AOP (4) Correlation (5) TR-PAC	(1) 1982MCM/GOL (2) 1992VEN/AMA (3) 1996ARM/SUN (4) 2000DEN/DEN (5) 2002SAN/MUR
benzenethiol, substituted 				
Y = 2-Cl	(1) 80.0	334.7	(1) AOP	(1) 1994BOR/ZHA(b)
3-Cl	(1) 80.1 (4) 80.3	335.1 335.8	(2) AOP	(2) 1992VEN/AMA
4-Cl	(1) 79.2 (4) 79.9 (5) 86.1±0.8	331.4 334.1 360.4±3.5	(3) AOP	(3) 1997ZHU/ZHA
4-Br	(1) 79.3 (2) 80.2	331.8 335.6	(4) Correlation	(4) 2000DEN/DEN
4-NH_2	(1) 69.8 (2) 70.0	292.0 292.9	(5) TR-PAC	(5) 2002SAN/MUR
2-Me	(1) 78.8	329.7		
3-Me	(1) 78.9 (4) 80.8	330.1 338.1		
4-Me	(1) 78.3 (2) 77.8 (3) 78.4 (4) 80.0 (5) 84.8±1.0	327.6 325.5 328.0 334.8 354.9±4.1		
4-MeO	(1) 76.9 (2) 76.2 (3) 78.6 (4) 78.7 (5) 83.3±1.0	321.7 318.8 328.9 329.3 348.5±4.0		
3-CF_3	(4) 80.8	338.1		
4-CF_3	(1) 80.9 (5) 86.0±0.9	338.5 359.9±3.9		

(continued)

Table 8.1 (continued) S–H BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
2-$MeCO_2$	(1) 78.7	329.3		
4-NO_2	(1) 81.4	340.6		
	(2) 81.6	341.4		
4-OH	(2) 76.0	318.0		
4-EtO	(4) 78.8	329.6		
4-tBu	(4) 80.7	337.7		
2,4,6-Me_3	(4) 80.4	336.6		
benzoylthiolate, substituted 				
Y = H	87.4	365.7	AOP	2000ZHA/LIN
CH_3	87	364.0		
CH_3O	87	364.0		
CF_3	86	359.8		
CN	86	359.8		
phenylmethane-1-thiol $PhCH_2S$–**H** $\Delta_f H^o(R)$ = 58.9 (246.4)	(1) 86.9 (2) 87.8	363.6 367.4	(1) AOP (2) Correlation	(1) 1994BOR/ZHA(b) (2) 1996DEN
naphthalenethiol 				
H–S at site 1	(2) 78.5	328.4	(1) AOP	(1) 1994BOR/ZHA(b)
2	(1) 77.9	325.9	(2) Correlation	(2) 2000DEN/DEN
	(2) 78.1	326.8		

thio-α-tocopherol 	80.0	334.7	Correlation	2000DEN/DEN

8.2 S–S bonds

Table 8.2 S–S BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
hydrogen disulfide **HS**–SH	64.7±1	270.7±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
methanehydrodifulfide CH_3S–**SH**	65.0	272.0	Derived	1999ARM
alkylhydrodifulfide RS–**SH**	65.2	272.8	Derived	1999ARM
dimethyl disulfide **CH_3S**–SCH_3	(1) 64 (2) 62.9±2.6 (3) **65.2±0.9**	267.8 263.2±10.9 **272.8±3.8**	(1) Electrochem. (2) Mol. beam (3) Resonance fluorescence	(1) 1992NUZ (2) 1988PEN/CAO (3) 1992NIC/KRE
diethyl disulfide **C_2H_5S**–SC_2H_5	66.1	276.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dipropyl disulfide **C_3H_7S**–SC_3H_7	66.2	277.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dialkyl disulfide **RS**–SR	66.2	277.0	Derived	1999ARM

(continued)

Table 8.2 (continued) S–S BDEs

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
diphenyl disulfide **C_6H_5S**–SC_6H_5	(1) 47 (2) **51.2±3** (3) 55±2	196.6 **214.2±12.6** 230±8.4	(1) Electrochem. (2) Derived from $\Delta_f H^o$ in ref. (3) AOP	(1) 1992NUZ (2) 1986PED/NAY (3) 1991BAU/FAS
hydrogen trisulfide **HS**–SSH	54.4±4	227.6±16.7	Derived	1978BEN
hydrogen tetrasulfide **HSS**–SSH	44.6±5	186.6±20.9	Derived	1978BEN
methyl methyl disulfanyl dissulfide **MeSS**–SSMe	32.9	137.7	Derived	1986HAW/GRI
ethyl ethyl disulfanyl dissulfide **EtSS**–SSEt	32.8	137.2	Derived	1986HAW/GRI
iso-propyl iso-propyl disulfanyl dissulfide **iPrSS**–SSPr	32.0	133.9	Derived	1986HAW/GRI
tert-butyl tert-butyl disulfanyl dissulfide **tBuSS**–SStBu	32.4	135.6	Derived	1986HAW/GRI

8.3 S–C bonds

Table 8.3 S–C BDEs

The broken bonds (**boldface** = dissociated group) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
Carbon disulfide **S**=CS	(1) 102.9±3 at 0K (2) **94.2**	430.5±12. 6 at 0K **394.1**	(1) MS (2) Derived from $\Delta_f H^o$ in ref.	(1) 1980MIL/ERE (2) 2002CRC
carbon oxysulfide **S**=CO	73.7	308.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
methanethiol **HS**—CH_3	(1) 74±1.5 (2) **74.7±1**	309.6±6.3 **312.5±4.2**	(1) Review (2) Resonance fluorescence	(1) 1978BEN (2) 1992NIC/KRE
ethanethiol **HS**–C_2H_5	73.6±0.5	307.9±2.1	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-propanethiol **HS**—nC_3H_7	74.2±0.7	310.5±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-propanethiol **HS**–iC_3H_7	73.4±0.9	307.1±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-butanethiol **HS**–nC_4H_9	73.9±0.7	309.2±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-butanethiol **HS**–sC_4H_9	73.5±0.7	307.5±2.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2-methyl-1-propanethiol **HS**–iC_4H_9	74.1±1.1	310.0±4.6	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

(continued)

Table 8.3 (continued) S–C BDEs

The broken bonds (**boldface** = dissociated group) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
2-methyl-2-propanethiol **HS**–tC_4H_9	72.0±0.9	301.2±3.8	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
cyclopentanethiol **HS**–c-C_5H_9	71.0±1.2	297.1±5.0	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-pentanethiol **HS**–nC_5H_{11}	73.5±1.5	307.5±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
2-methyl-2-butanethiol **HS**–C$(CH_3)2(C_2H_5)$	71.6±1.5	299.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
2,2-dimethyl-1-propanethiol **HS**–neoC5H_{11}	73.7±2.0	308.4±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
1-hexanethiol **HS**–nC_6H_{13}	73.2±1.5	306.3±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
benzenethiol **HS**–C_6H_5	86.5±2	361.9±8.4	Review	1978BEN
cyclohexanethiol **HS**–cC_6H_{11}	72.9±1.4	305.0±5.9	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
benzenemethanethiol **HS**–$CH_2C_6H_5$	60.4±1.8	252.7±7.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
thioacetic acid **HS**–C(O)CH_3	73.6±1.5	307.9±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC

dimethyl sulfide **CH_3S**–CH_3	(1) 77.2±2 (2) **73.6±0.8**	323.0±8.4 **307.9±3.3**	(1) Pyrolysis (2) Resonance fluorescence	(1) 1977COL/BEN (2) 1992NIC/KRE
ethyl methyl sulfide **CH_3S**–C_2H_5	72.4±1	302.9±4.2	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl methyl sulfide **C_2H_5S**–CH_3	73.4±1.5	307.1±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl propyl sulfide **CH_3S**–C_3H_7	73.3±1.5	306.7±6.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl propyl sulfide **C_3H_7S**–CH_3	73.9±1.5	309.2±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iso-propyl methyl sulfide **CH_3S**–iC_3H_7	72.4±1.5	302.9±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butyl methyl sulfide **CH_3S**–C_4H_9	72.8±1.5	304.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl methyl sulfide **CH_3S**–tC_4H_9	70.4±1.5	294.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl propyl sulfide **C_2H_5S**–C_3H_7	72.9±1.5	305.0±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
ethyl propyl sulfide **C_3H_7S**–C_2H_5	72.5±1.5	303.3±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC
ethyl isopropyl sulfide **C_2H_5S**–iC_3H_7	73.4±1.5	307.1±6.3	Derived from $\Delta_f H^o$ in ref.	2002CRC

(continued)

Table 8.3 (continued) S-C BDEs

The broken bonds (**boldface** = dissociated group) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
cyclopentyl methyl sulfide **CH_3S**–c-C_5H_9	70.6±1.5	295.4±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl pentyl sulfide **CH_3S**–C_5H_{11}	71.9±1.5	300.8±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
diethyl sulfide **C_2H_5S**–C_2H_5	72.5±1.5	303.3±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
ethyl butyl sulfide **C_2H_5S**–C_4H_9	73.0±1.5	305.4±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
tert-butyl ethyl sulfide **C_2H_5S**–tC_4H_9	71.1±1.5	297.5±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
dipropyl sulfide **C_3H_7S**–C_3H_7	72.8±1.5	304.6±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl phenyl sulfide **CH_3S**–C_6H_5	85.4±1.5	357.3±6.3	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl phenyl sulfide **C_6H_5S**–CH_3	(1) 69.4±2 (2) **66.5±2.5**	290.4±8.4 **278.2±10.5**	(1) VLPP (2) Derived from $\Delta_f H^o$ in ref.	(1) 1977COL/BEN (2) 1994PED
ethyl phenyl sulfide **C_2H_5S**–C_6H_5	84.6±2	354.0±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY

ethyl phenyl sulfide C_2H_5–**SC_6H_5**	64.5±1.5	269.9±6.3	Derived from Δ_fH^o in ref.	1994PED
benzyl methyl sulfide **CH_3S**–CH_2Ph	61.4±2	256.9±8.4	VLPP	1977COL/BEN
diphenyl sulfide **C_6H_5S**–C_6H_5	(1) 78.3±2.5 (2) 76±2	327.6±10.5 318±8.4	(1) Derived from Δ_fH^o in ref. (2) AOP	(1) 1986PED/NAY (2) 1991BAU/FAS
dimethyl disulfide **CH_3**–$SSCH_3$	56.6	236.8	AE	1986HAW/GRI
ethyl methyl disulfide **C_2H_5**–$SSCH_3$	56.2	235.1	AE	1986HAW/GRI
iso-propyl methyl disulfide **iC_3H_7**–$SSCH_3$	54.5	228.0	AE	1986HAW/GRI
methyl tert-butyl disulfide **tC_4H_9**–$SSCH_3$	52.6	220.1	AE	1986HAW/GRI
methanesulfenic acid HOS–**CH_3**	68.1±3	284.9±12.6	Derived from Δ_fH^o in ref.	1996HUN/SHE
methanesulfonic acid $HOSO_2$–**CH_3**	77.5±3	324.3±12.6	Derived from Δ_fH^o in ref.	2000GUT/GAL
dimethyl sulfone CH_3SO_2–**CH_3** $\Delta_fH^o(CH_3SO_2)$ = –57.2 (–239.3)	66.8	279.5	Iodination	1971SOL/BEN

(continued)

Table 8.3 (continued) S–C BDEs

The broken bonds (**boldface** = dissociated group) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
methyl sulfone radical **CH_3**–SO_2	21.4	89.5	Derived from $\Delta_f H^o$ in ref.	1971SOL/BEN
ethyl methyl sulfone CH_3SO_2–**C_2H_5**	68.9±2	288.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
iso-propyl methyl sulfone CH_3SO_2–**iC_3H_7**	67.5±2	282.4±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
allyl methyl sulfone H_3CSO_2–**C_3H_5**	55.0±2.5	230.1±10.5	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
butyl methyl sulfone H_3CSO_2–**C_4H_9**	71.3±2	298.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl tert-butyl sulfone H_3CSO_2–**tC_4H_9**	67.6±2	282.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methyl phenol sulfone H_3CSO_2–**C_6H_5**	82.3±2	344.3±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
benzyl methyl sulfone CH_3SO_2–**CH_2Ph**	56.2±2	235.1±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
methylthiocarbonitrile CH_3S–**CN**	97.0±2	405.8±8.4	Derived from $\Delta_f H^o$ in ref.	1986PED/NAY
S-ethyl thioacetate **C_2H_5S**–$C(O)CH_3$	76.2±2	318.8±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC

S-propyl thioacetate $\mathbf{C_3H_7S}$–C(O)CH_3	76.5±2.0	320.1±8.4	Derived from $\Delta_f H^o$ in ref.	1994PED
pentafluorosulfur trifluoromethane $\mathbf{F_5S}$–CF_3	93.7±10.3 at 0 K	392.0±43 at 0 K	Threshold photoelectron	2001CHI/KEN
methanedisulfur radical CH_3–**SS**	49.4	206.7	Derived from $\Delta_f H^o$ in ref.	1986HOW/GRI
ethanedisulfur radicals C_2H_5–**SS**	48.7	203.8	Derived from $\Delta_f H^o$ in ref.	1986HOW/GRI
propane-2-disulfur radical iC_3H_7–**SS**	48.4	202.5	Derived from $\Delta_f H^o$ in ref.	1986HOW/GRI
2-methylpropane-2-disulfur radical tC_4H_9–**SS**	46.9	196.2	Derived from $\Delta_f H^o$ in ref.	1986HOW/GRI

8.4 S–halogen and S–P bonds

Table 8.4 S–Halogen BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
sulfur hexafluoride **F**–SF_5	(1) 92.2	385.8	(1) High pressure MS	(1) 1990SIE/AUS
	(2) **100.4±2.4**	420±10	(2) SPST	(2) 1992TSA/HER
chloromethylsulfone **Cl**–SO_2CH_3	(1) 70.3 (2) 70	(1) 294 (2) 293	PAC	(1) 1994CHA/GRI (2) 1999LAA/MUL

(continued)

Table 8.4 (continued) S–Halogen BDEs

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
chlorophenylsulfone **Cl**–SO_2Ph	(1) 70.5 (2) 71	(1) 295.0 (2) 297.0	PAC	(1) 1994CHA/GRI (2) 1999LAA/MUL
iodothio **I**–SH	49.4±2	206.7±8.4	Kinetics	1979HWA/BEN(b)
iodosulfoxide **I**–SO	130.1±1.5 at 0K	544.3±6.3 at 0 K	Spectroscopy	1971OKA
iodomethylthio **I**–SCH_3	49.3±1.7	206.3±7.1	VLPP	1983SHU/BEN
trifluorophosphino-1-thione **S**=PF_3	100	418.4	Review	1973BEN
trichlorophosphino-1-thione **S**=PCl_3	68	284.5	Review	1973BEN
tribromophosphino-1-thione **S**=PBr_3	94	393.3	Review	1973BEN

chapter nine

Tabulated BDEs of Si–, Ge–, Sn–, P– and Se–X bonds

9.1 Si–X bonds

Table 9.1 Si–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
silane	(1) 90.3±1.2	377.8±5.0	(1) Iodination	(1) 1981DON/WAL
SiH_3–**H**	(2) 91.8±0.5	384.1±2.1	(2) PIMS detect.	(2) 1991SEE/FEN
$\Delta_f H^o(R)$ = 47.9±0.6	(3) **91.7±0.5**	**383.7±2.1**	(3) Recommended	(3) 1994BER/ELL
(200.4±2.5)	(4) 91.5±2	382.8±8.4	(4) Review	(4) 1995CHA
	(5) 91.8±0.5	384±2	(5) Review	(5) 1998BEC/WAL
methyl saline	(1) 89.6±2	374.9±8.4	(1) Iodination	(1) 1989WAL
$MeSiH_2$–**H**	(2) 92.3±3	386.2±12.6	(2) Review	(2) 1995CHA
$\Delta_f H^o(R)$ = 33.7±1.5	(3) **92.7±1.2**	**388±5**	(3) Revised	(3) 1998BEC/WAL
(141±6)				
dimethylsaline	(1) 89.4±2	374.0±8.4	(1) Iodination	(1) 1989WAL
Me_2SiH–**H**	(2) **93.5±1.2**	**391±5**	(2) Revised	(2) 1998BEC/WAL
$\Delta_f H^o(R)$ = 18.6±1.5				
(78±6)				
trimethylsaline	(1) 90.3±1.4	377.8±5.9	(1) Iodination	(1) 1989WAL
Me_3Si–**H**	(2) 95.0±0.5	397.5±2.1	(2) Flash photolysis	(2) 1994KAL/GUT

(continued)

Table 9.1 (continued) Si–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
$\Delta_f H^o$(R) = 3.6±1.7 (15±7)	(3) 92.0	385	(3) VLPP	(3) 1994BUL/WAL
	(4) **94.6±1.7**	**396±7**	(4) Revised	(4) 1998BEC/WAL
Me_3Si–**D**	(5) 93.0	389.1	(5) Kinetics	(5) 1981ELL/POT
disilane H_5Si_2–**H** $\Delta_f H^o$(R) = 55.9±2.0 (234±8)	(1) 86.3±2	361.1±8.4	(1) Iodination	(1) 1989WAL
	(2) **89.1±2**	**373±8**	(2) Revised	(2) 1998BEC/WAL
3-ethyl-silapentane $(C_2H_5)_3Si$–**H**	(1) 90.1	377.0	(1) PAC	(1) 1987KAM/HAW
	(2) 95.1	397.9	(2) Review	(2) 1995CHA
	(3) 96	401.7	(3) PAC, revised	(3) 1999LAA/MUL
	(4) **94.6±1**	**396±4**	(4) Review	(4) 1998BEC/WAL
pentamethyl disilane $(CH_3)_3Si(CH_3)_2Si$–**H**	(1) 85.3±2	356.9±8.4	(1) PAC	(1) 1987KAM/HAW
	(2) 90.3	377.8	(2) Review	(2) 1995CHA
	(3) 91	380.7	(3) PAC, revised	(3) 1999LAA/MUL
	(4) **89.9±1**	**376±4**	(4) Review	(4) 1998BEC/WAL
3(1,1-dimethyl-1-silaethyl)-2,2,4,4,-tetramethyl-2,3,4-trisilapentane $[(CH_3)_3Si]_3Si$–**H**	(1) 79.0	330.5	(1) PAC	(1) 1987KAM/HAW
	(2) 83.9	351.0	(2) Review	(2) 1995CHA
	(3) 84.0	351.5	(3) PAC, revised	(3) 1999LAA/MUL
	(4) **83.7±1**	**350±4**	(4) Review	(4) 1998BEC/WAL
2,2,3,4,4-pentamethyl-3-silapentane $(tBu)_2MeSi$–**H**	89.1	372.8	Correlation	1998DEN
3-(tert-butyl)-2,2,4,4-tetramethyl-3-silapentane $(tBu)_3Si$–**H**	86.6	362.3	Correlation	1998DEN

1-phenyl-silaethane $C_6H_5SiH_2$–**H** $\Delta_fH^o(R)$ = 62.1 (260)	(1) 88.2±1.2 (2) 90.1 (2) **91.3±1.2**	369.0±5 377.0 **382±5**	(1) Iodination (2) Review (3) Revised	(1) 1989WAL (2) 1995CHA (3) 1998BEC/WAL
trimethylthiosilamethane $(CH_3S)_3Si$–H	(1) 82.5 (2) 87.4 (3) **87.0**	345.2 365.7 **364.0**	(1) PAC (2) Review (3) PAC, revised	(1) 1992CHA/GUE (2) 1995CHA (3) 1999LAA/MUL
triisopropylthiosilamethane $(iPrS)_3Si$–**H**	(1) 85.6 (2) **90.0**	358.2 **376.6**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
phenyl methyl silamethane, substituted R_1R_2MeSi–**H**				
R_1 = Ph R_2 = H	(1) 91.3±3.1	382.0±13	(1) ICR	(1) 1989WET/SAL
Ph F	(2) 92.1	385.4	(2) Correlation	(2) 1998DEN
Ph Cl	(2) 90.0	376.6		
Ph C_6F_5	(2) 89.7	375.5		
Ph Ph_3Si	(2) 83.1	347.7		
Ph $tBuCH_2$	(2) 87.5	366.2		
Me 3-CF_3–C_6H_4	(2) 87.1	364.2		
1-Np C_6H_5	(2) 87.2	365.0		
1-Np 3-F–C_6H_4	(2) 88.2	369.2		
1-Np 3-MeO–C_6H_4	(2) 87.5	366.2		
1-Np 3-CF_3–C_6H_4	(2) 88.3	369.6		
1-Np 3-Me–C_6H_4	(2) 86.9	363.6		
1-Np 4-CF_3–C_6H_4	(2) 88.6	370.7		
1-Np 4-MeO–C_6H_4	(2) 86.6	362.4		
dimethyl phenyl silamethane $PhMe_2Si$–**H**	(1) 85.6 (2) 88.7 (3) **90.1±1.7**	354.0 371.0 **377±7**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL

(continued)

Table 9.1 (continued) Si–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
diphenyl silamethane Ph_2SiH–**H**	(1) 86.0 (2) 87.7 (3) **90.6±1.7**	359.8 366.8 **379±7**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
diphenyl methyl silamethane Ph_2MeSi–**H**	(1) 81.7 (2) 87.5 (3) **86.3±2.4**	341.8 366.2 **361±10**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
triphenyl silamethane, substituted R_3Si–**H** R = C_6H_5	(1) 84.1 (2) 86.4 (3) **88.7±0.5**	351.9 361.8 **371±2**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
3-CF_3–C_6H_4	(2) 89.3	373.6		
trifluorosilane SiF_3–**H** $\Delta_f H^o$(R) = –235.9±4.8 (–987±20)	(1) 100.1±1.2 (2) **103.2±1.2**	418.8±5.0 **432±5**	(1) Iodination (2) Revised	(1) 1989WAL (2) 1998BEC/WAL
trichlorosilane $SiCl_3$–**H** $\Delta_f H^o$(R) = –77±2 (–322±8)	(1) 91.3±1.2 (2) **94.4±1.2**	382.0±5.0 **395±5**	(1) Iodination (2) Revised	(1) 1989WAL (2) 1998BEC/WAL
tribromosilane $SiBr_3$–**H**	79.8±2	334.0±8.0	Derived from $\Delta_f H^o$ in ref.	2002CRC
methyl silane SiH_3–**CH_3**	89.6±1.2	375±5	Derived	1998BEC/WAL

2-silapropane $MeSiH_2$–**CH_3**	90.1±1.7	377±7	Derived	1998BEC/WAL
trimethylsaline Me_2SiH–**CH_3**	92.5±1.7	387±7	Derived	1998BEC/WAL
tetramethylsaline Me_3Si–**CH_3**	(1) 91.6 (2) **94.2±2**	383.0 **394±8**	(1) VLPP (2) Derived	(1) 1994BUL/WAL (2) 1998BEC/WAL
trimethyl sec-butylsilane Me_3Si–**sBu**	99	414.2	Pyrolysis	1980DAV/WOO
trimethyl allylsilane Me_3Si–**C_3H_5**	70	292.9	Pyrolysis	1980DAV/WOO
disilane SiH_3–**SiH_3**	76.7±1	321±4	Derived	1998BEC/WAL
trisilane **SiH_3**–Si_2H_5	74.8±2	313±8	Derived	1998BEC/WAL
tetrasilane **H_5Si_2**–Si_2H_5	73.1	306	Derived	1998BEC/WAL
hexamethyl disilane **Me_3Si**–$SiMe_3$	(1) 80.5 (2) **79.3±2.9**	336.8 **332±12**	(1) Pyrolysis (2) VLPP	(1) 1975DAV/HOW (2) 1994BUL/WAL
hexaphenyl disilane **Ph_3Si**–$SiPh_3$	88.0	368.2	Derived	1981WAL
2-methyl-2-silapropan-2-ol Me_3Si–**OH**	132.6±2	555±8	Derived	1998BEC/WAL

(continued)

Table 9.1 (continued) Si–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o(R)$, kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
1-methoxy-1,1-dimethyl-1-silaethane Me_3Si–**OMe**	122.6±2.6	513±11	Derived	1998BEC/WAL
1-ethoxy-1,1-dimethyl-1-silaethane Me_3Si–**OEt**	122.4±2.6	512±11	Derived	1998BEC/WAL
2,2,6,6-tetramethyl-4-oxa-3,5-disilapentane Me_3Si–**OSiMe$_3$**	136.0	569	Derived	1998BEC/WAL
nitrososilane H_3Si–**NO** D_3Si–**NO**	37.8±1.4 38.4±1.4	158.2±5.7 160.8±5.7	Laser photolysis MS	1997KRA/KAL
nitroso trimethylsilane Me_3Si–**NO**	44.8±1.0	187.4±4.2	Laser photolysis, MS detect.	1995KRA/NII
(1,1-dimethyl-1-silaethyl)-methylamine Me_3Si–**NHMe**	100.1±2	412±8	Derived	1998BEC/WAL
(1,1-dimethyl-1-silaethyl)-dimethylamine Me_3Si–**NMe$_2$**	97.5±2	408±8	Derived	1998BEC/WAL
tri(1,1-dimethyl-1-silaethyl)-amine Me_3Si–**N(SiMe$_3$)$_2$**	108.7	455	Derived	1998BEC/WAL

fluorosilane SiH_3–**F**	152.5±1.2	638±5	Derived	1998BEC/WAL
trimethyl fluorosilane Me_3Si–**F**	~159.9±4.8	669±20	Derived	1989WAL
tetrafluorosilane SiF_3–**F**	166.6±1.5	697±6	Derived	1998BEC/WAL
chlorosilane SiH_3–**Cl**	109.5±1.7	458±7	Derived	1998BEC/WAL
trimethyl chlorosilane Me_3Si–**Cl**	112.8±2	472±8	Derived	1989WAL
tetrachlorosilane $SiCl_3$–**Cl**	110.4±2.2	462±9	Derived	1998BEC/WAL
bromosilane SiH_3–**Br**	89.9±2.2	376±9	Derived	1998BEC/WAL
trimethyl bromosilane Me_3Si–**Br**	96.0±2	402±8	Derived	1989WAL
tetrabromosilane $SiBr_3$–**Br**	89.9±5.3	376±22	Derived	1998BEC/WAL
iodosilane SiH_3–**I**	71.5±2	299±8	Derived	1998BEC/WAL
trimethyl iodosilane Me_3Si–**I**	(1) 76.9 (2) **76.7**±**2**	321.7 **320.9**±**8.4**	(1) UV spectrom. (2) Derived	(1) 1979DON/WAL (2) 1989WAL

(continued)

Table 9.1 (continued) Si–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
tetraiodosilane SiI_3–**I**	67.9±6.2	284±26	Derived	1998BEC/WAL
2-silaeth-1-ene SiH_2=**CH_2**	34.9±1	146±4	Review	1998BEC/WAL
2-silapro-1-ene MeHSi=**CH_2**	36.8±2.9	154±12	Review	1998BEC/WAL
2-methyl-2-silapro-1-ene Me_2Si=**CH_2**	38.5±2.9	161±12	Review	1998BEC/WAL
disilene SiH_2=**SiH_2**	27.0±2	113±8	Review	1998BEC/WAL
silaforaldehyde SiH_2=**O**	61.2±6	256±25	Review	1998BEC/WAL

9.2 Ge–X bonds

Table 9.2 Ge–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
germane GeH_3–**H** $\Delta_f H^o$(R) = 53±2 (221.8±8.4)	(1) 78.0±1	326.4	(1) VLPP	(1) 1987AGR/SET
	(2) 82.6±2.4	345.6±10.0	(2) VLPP	(2) 1983NOB/WAL
	(3) **83.4±2**	**348.9±8.4**	(3) Recommend.	(3) 1994BER/ELL
	(4) 85.6±2.1	358.2±8.8	(4) FT-ICR	(4) 1993DEC/GAL
	(5) 82.5	345.2	(5) Electron affinity	(5) 2001MOR/RIV

trimethylgermane Me_3Ge–**H**	(1) 81.7±2.4 (2) 82 (3) 81.6±0.5 (4) 79.8±3.5 (5) **87**	341.8±10.0 343.1 341.4±2.1 333.9±14.6 **364**	(1) VLPP (2) AE (3) PAC (4) Electron photodetach. (5) PAC, revised	(1) 1979DON/WAL (2) 1979JAC (3) 1991CLA/GRI (4) 1995BRI/SAL (5) 1999LAA/MUL
triethyl germane $(C_2H_5)_3Ge$–**H**	(1) 82.3 (2) **86.0**	344.3 **359.8**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
tri-tert-butyl germane $(tBu)_3Ge$–**H**	(1) 82.6 (2) **88.0**	345.6 **368.2**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
3-(1,1-dimethyl-1-silaethyl)-3-germa-2,2,4,4-tetramethyl-2,4-disilapentane $(Me_3Si)_3Ge$–**H**	73.1	305.8	Correlation	2002DRO/DEN
phenylgermane, substituted (2,4,6-Me_3–C_6H_2)GeH_2–**H**	80.7	337.5	Correlation	2002DRO/DEN
diphenylgermane, substituted (2,4,6-Me_3–C_6H_2)$_2$GeH–**H**	80.5	336.8	Correlation	2002DRO/DEN
2-germa-1-phenylfromtane $(PhCH_2)(C_2H_5)GeH$–**H**	81.6	341.6	Correlation	2002DRO/DEN
2-germa-1,3-diphenyl-2-benzylpropane $(PhCH_2)_3Ge$–**H**	77.7	324.9	Correlation	2002DRO/DEN
phenyl germane PhH_2Ge–**H**	(1) 79.2 (2) **86.0**	331.4 **359.8**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL

(continued)

Table 9.2 (continued) Ge–X BDEs

The broken bonds (**boldface** = dissociated atom) $\Delta_f H^o$(R), kcal/mol (kJ/mol)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
diphenyl germane Ph_2HGe–**H**	(1) 79.5 (2) **85.0**	332.6 **355.6**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
triphenyl germane Ph_3Ge–**H**	(1) 80.2 (2) **86.0** (3) 77.1	335.6 **359.8** 322.5	(1) PAC (2) PAC, revised (3) Correlation	(1) 1991CLA/GRI (2) 1999LAA/MUL (3) 2002DRO/DEN
methoxygermane $H_2Ge(OMe)$–**H**	81.5	341.0	Electron affinity	2001MOR/RIV
dimethoxygermane $HGe(OMe)_2$–**H**	82.6	345.6	Electron affinity	2001MOR/RIV
digermane H_3Ge–**GeH_3**	67.2±3	281.2±8.4	Derived from $\Delta_f H^o$ in ref.	2002CRC

9.3 *Sn–X bonds*

Table 9.3 Sn–X BDEs

The broken bonds (**boldface** = dissociated atom or group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
trimethylstannane Me_3Sn–H	(1) 74 (2) 75±3.5	309.6 313.8±14.6	(1) PAC (2) Electron photodetach.	(1) 1991CLA/GRI (2) 1995BRI/SAL
	(3) **78.0** (4) 76.1 (5) 77±4	**326.4** 318.5 322±17	(3) PAC, revised (4) Correlation (5) Derived	(3) 1999LAA/MUL (4) 2002DRO/DEN (5) 2002BEC/BOG

tributylstannane $(nBu)_3Sn$–**H**	(1) 73.7±2.0 (2) **78.0**	308.4±8.4 **326.4**	(1) PAC (2) PAC, revised	(1) 1986BUR/MAJ (2) 1999LAA/MUL
triphenylstannane Ph_3Sn–**H**	70.4 71.3	294.6 298.3	Correlation	2002DRO/DEN
2,2-dimethyl-2-stannapropane Me_3Sn–**Me**	64.0	267.8	Derived	1988GRI/KAM
2,2-dimethyl-2-stannabutane Me_3Sn–**Et**	60.0	251.0	Derived	1988GRI/KAM
2,2,3-trimethyl-2-stanna-butane Me_3Sn–**iPr**	55.4	231.8	Derived	1988GRI/KAM
2,2,3,3-tetramethyl-2-stanna-butane Me_3Sn–**tBu**	50.4	310.9	Derived	1988GRI/KAM

9.4 P–X bonds

Table 9.4 P–X BDEs

The broken bonds (**boldface** = dissociated atom or group)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
phosphine H_2P–**H**	83.9±0.5	351.0±2.1	Recommended	1994BER/ELL
octylphosphine $CH_3(CH_2)_7PH$–**H**	89.7	375.3	PAC	1999LAA/MUL
ethylphosphine C_2H_5PH–**H**	89.7	375.3	MS	1969BOG/GRI

(continued)

Table 9.4 (continued) P–X BDEs

The broken bonds (**boldface** = dissociated atom or group)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
α-CN-proyulphosphine $NC(CH_2)_3PH$–**H**	89.2	373.4	Correlation	2002DRO/DEN
di(α-CN-proyul)phosphine $[NC(CH_2)_3]_2P$–**H**	88.3	369.5	Correlation	2002DRO/DEN
dibutylphosphine $[CH_3(CH_2)_3]_2P$–**H**	89.6	375.0	Correlation	2002DRO/DEN
diethylphosphine $(CH_3CH_2)_2P$–**H**	90.3	377.8	Correlation	2002DRO/DEN
dicyclohexylphosphine (cyclo-$C_6H_{11})_2P$–**H**	85.5 86.9	357.6 363.6	Correlation	2002DRO/DEN
diphosphine **H_2P**–PH_2	61.2	256.1	MS	1969MCA/LOS
tetrachlorodiphosphine **Cl_2P**–PCl_2	58	242.7	MS	1963SAN/MOS
tetraiododiphosphine **I_2P**–PI_2	73	305.4	MS	1969FIN/HAM
(diethylphosphino)diethyl-phosphine **$(C_2H_5)_2P$**–$P(C_2H_5)_2$	86	359.8	MS	1968GRI/BOG

9.5 *Se–X bonds*

Table 9.5 Se–X BDEs

The broken bonds (**boldface** = dissociated atom or group)	BDEs (**boldface** = recommended data; references in parentheses)		Methods (references in parentheses)	References
	kcal/mol	kJ/mol		
hydrogen selenide HSe–**H**	80.05±0.18	334.93±0.75	Recommend.	1994BER/ELL
benzeneselnol C_6H_5Se–**H**	78±4	326.4±16.7	ICR	1996LEE/LI

chapter ten

Tabulated BDEs in some inorganic compounds

Table 10.1 BDEs in Some Inorganic Compounds

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
H_2N–**H**	108.2±0.3	452.7±1.3	Recommend.	1994BER/ELL
HN–**H**	97.0	405.8	Derived from $\Delta_f H^o$ in ref.	1998NIST
N–**H**	≤81.0	≤338.9	Spectroscopy	2002CRC
H_2N–**NH_2**	67.4	282.0	Derived from $\Delta_f H^o$ in ref.	1998NIST
H–N_3	93.8	392.5	Derived from $\Delta_f H^o$ in ref.	2002CRC
H_2P–**H**	83.9±0.5	351.0±2.1	Recommend.	1994BER/ELL
HP–**H**	75.3	315.1	Derived from $\Delta_f H^o$ in ref.	1998NIST

(continued)

Table 10.1 (continued) BDEs in Some Inorganic Compounds

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
P–**H**	71.0	297.1	Spectroscopy	2002CRC
H_2P–**PH_2**	61.2	256.1	Derived from $\Delta_f H^o$ in ref.	2002CRC
F–PH_2	110.3±2.5	461.5±10.5	Derived from $\Delta_f H^o$ in ref.	2000FER/ALC
H_2As–**H**	76.3±0.2	319.2±0.8	Recommend.	1994BER/ELL
HAs–**H**	52.1	218.0	Derived from $\Delta_f H^o$ in ref.	1998NIST
As–**H**	65.5±0.9	274.1±3.8	PIMS	1988BER
H_2Sb–**H**	68.9±0.5	288.3±2.1	Recommend.	1994BER/ELL
H_3C–**H**	105.0±0.1	439.3±0.4	VLPP	1987DOB/BEN
H_2C–**H**	110.3	461.5	Derived from $\Delta_f H^o$ in ref.	1998NIST
HC–**H**	100.8	421.7	Derived from $\Delta_f H^o$ in ref.	1998NIST
C–**H**	80.9	338.5	Spectroscopy	2002CRC

H_3Si–**H**	91.7±0.5	383.7±2.1	Recommend.	1994BER/ELL
H_2Si–**H**	71.0±2	297.1±8.4	Derived	1989WAL
HSi–**H**	76.7	320.9	Derived	1989WAL
Si–**H**	69.8	292	Derived	1998BEC/WAL
H_3Ge–**H**	83.4±2.0	348.9±8.4	Recommend.	1994BER/ELL
Ge–**H**	≤76.9	≤321.7	Spectroscopy	1966KLY/LIN
HO–**H**	119.30±0.05	499.15±0.21	Recommend.	1994BER/ELL
O–**H**	102.20	426.60	Spectroscopy	2002CRC
HS–**H**	91.2±0.7	381.6±2.9	Recommend.	1994BER/ELL
S–**H**	82.3±2.3	344.3±9.6	Spectroscopy	2002CRC
HSe–**H**	80.05±0.18	334.93±0.75	Recommend.	1994BER/ELL
Se–**H**	~43.0	~180	Spectroscopy	2002CRC
HTe–**H**	66.2±1.2	277.0±5.0	Recommend.	1994BER/ELL
Te–**H**	64.1	268.2	Spectroscopy	2002CRC

(continued)

Table 10.1 (continued) BDEs in Some Inorganic Compounds

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
N_2H_3–**H**	87.5	366.1	Derived from $\Delta_f H^o$ in ref.	1998NIST
N_2H_2–**H**	44.8	187.4	Derived from $\Delta_f H^o$ in ref.	1998NIST
OS–**H**	54.3	227.2	Derived from $\Delta_f H^o$ in ref.	1998NIST
O_2S–**H**	34.2	143.5	Derived from $\Delta_f H^o$ in ref.	1998NIST
ON–**H**	46.7	195.4	Derived from $\Delta_f H^o$ in ref.	1998NIST
O_2N–**H**	79.0	330.5	Derived from $\Delta_f H^o$ in ref.	1998NIST
F_2N–**F**	60.6	253.6	Derived from $\Delta_f H^o$ in ref.	1998NIST
FN–**F**	58.8	246.0	Derived from $\Delta_f H^o$ in ref.	1998NIST
N–**F**	82.0	343.1	Spectroscopy	1979HUB/HER
O–N	150.70±0.03	630.53±0.13	Spectroscopy	2002CRC

O–NO	72.9	305.0	Review	1965BEN
O–NO_2	47.3±0.8 at 0 K	197.9±3.3 at 0 K	Photodissocn.	1993DAV/KIM
ON–ON	9.7±0.5	40.6±2.1	Review	1976BEN
ON–NO_2	8.8	36.8	Derived from $\Delta_f H^o$ in ref.	2002CRC
O_2N–NO_2	13.2	55.2	Derived from $\Delta_f H^o$ in ref.	2002CRC
O_2N–ONO_2	24.6	102.9	Derived from $\Delta_f H^o$ in ref.	2002CRC
O–N_2	40.0	167.4	Derived from $\Delta_f H^o$ in ref.	2002CRC
HO–NO	49.4	206.7	Review	1982MCM/GOL
HO–NO_2	49.3	206.3	Review	1982MCM/GOL
HOO–NO_2	23±2	96.2±8.4	Derived	1978BAL/GOL
O=O	119.11±0.04	498.36±0.17	Spectroscopy	2002CRC
S=S	101.65	425.30	Spectroscopy	2002CRC
O=S	123.78±0.01	517.90±0.04	Spectroscopy	2002CRC

(continued)

Table 10.1 (continued) BDEs in Some Inorganic Compounds

The broken bonds (**boldface** = dissociated atom)	BDEs (**boldface** = recommended data; references in parentheses) kcal/mol	kJ/mol	Methods (references in parentheses)	References
N≡N	225.94±0.14	945.33±0.59	Spectroscopy	2002CRC
C–C	143.75	601.45	Spectroscopy	2002CRC
C–N_2	29.5±0.8	123.4±3.3	Derived from $\Delta_f H^o$ in ref.	2000BIS/HOO

chapter eleven

Heats of formation of atoms, inorganic and organic radicals

11.1 Gaseous atoms

Table 11.1 Heats of Formation of Gaseous Atoms

	$\Delta_f H^o$			$\Delta_f H^o$	
Atom	kcal/mol	kJ/mol	Atom	kcal/mol	kJ/mol
Ag	68.1±0.2	284.9±0.8	Fe	99.30	415.47
Al	78.87±0.96	330.0±4.0	Ga	65.00	271.96
As	53.53±0.53	223.97±2.22	Ge	89±2	372.4±8.4
Au	20.0±1.3	83.7±5.4	H	52.103±0.001	217.998±0.006
B	133.84	560.00	Hf	147.80	618.40
Ba	42.801	179.08	Hg	14.67±0.01	61.38±0.04
Be	77.438	324.00	I	25.516±0.01	106.76±0.04
Bi	27.7±1.0	95.0±4.2	In	48.2±2.2	201.7±9.2
Br	26.735	111.86	Ir	122.92±0.50	514.30±2.09
C	171.29±0.11	716.68±0.45	K	21.27	89.00
Ca	42.495	177.80	La	92.16±0.68	385.59±2.85
Cd	26.721±0.048	111.80±0.20	Li	38.074	159.30
Cl	28.992±0.002	121.301±0.008	Mg	35.158	147.10
Co	101.98	426.68	Mn	67.701	283.26
Cr	95.0	397.48	Mo	157.50	658.98
Cs	18.28	76.50	N	112.97±0.096	472.68±0.40
Cu	80.688	337.60	Na	25.645	107.30
F	18.97±0.072	79.38±0.30	Nb	175.20	733.04

(continued)

Table 11.1 (continued) Heats of Formation of Gaseous Atoms

	$\Delta_f H^o$			$\Delta_f H^o$	
Atom	kcal/mol	kJ/mol	Atom	kcal/mol	kJ/mol
Ni	102.80	430.12	Si	107.55	450.00
O	59.555±0.024	249.18±0.10	Sn	71.99±0.36	301.21±1.5
Os	164.1±5.0	686.6±20.9	Sr	39.197	164.00
P	75.619	316.39	Ta	186.90	782.00
Pb	46.654	195.20	Te	47.0	196.6
Pd	77.44±0.50	324.01±2.09	Th	144±1	602.5±4.2
Pt	86.10	360.24	Ti	113.20	473.63
Rb	19.34	80.92	Tl	34.5±1.7	144.3±7.1
Rh	106.74±0.50	446.60±2.09	U	127±2	531.4±8.4
Ru	129.47	541.70	V	123.20	515.47
S	66.200	276.98	W	203.40	851.03
Sb	38.5±1.5	161.1±6.3	Y	93.62±0.57	391.71±2.38
Sc	86.0±1.1	358.8±4.6	Zn	31.171	130.42
Se	7.7±1.4	32.2±5.9	Zr	145.80	610.03

Data resource: http://webbook.nist.gov

11.2 Small inorganic radicals in the gas phase

Table 11.2 Heats of Formation of Small Inorganic Radicals

	$\Delta_f H^o(R)$		
Inorganic radicals	kcal/mol	kJ/mol	References
ON	21.58	90.29	1998CHA
NO_2	7.91	33.10	1998CHA
ONOO	19.8	82.8	1993DAV/KIM
sym-NO_3	15.8	66.1	1976BEN
N_2O	19.61	82.05	1998CHA
NH	90.0	376.56	1998CHA
NH_2	45.1±0.3	188.7±1.3	1994BER/ELL
HNO	27.0	113.0	1996DIX

N_3	112±5	468.6±20.9	1982MCM/GOL
N_2H_3	58.2	78.2	1988GRE/COL
(Z)-N_2H_2	50.9	212.97	1998CHA
NF_2	10.1	42.26	1998CHA
NF	50	209.2	1979HUB/HER
HNO	23.8	99.58	1998CHA
FNO	–15.7	–65.69	1998CHA
ClNO	12.36	51.71	1998CHA
BrNO	19.63	82.13	1998CHA
INO	26.8	112.13	1998CHA
NCN	111.1±0.7	464.8±2.9	1999BIS/CHO
OH	9.40±0.05	39.33±0.21	1994BER/ELL
SH	34.18±0.68	143.01±2.85	1994BER/ELL
SSH	27.6±3.5	115.5±14.6	1993OHA/DEP
SO	1.2	5.01	1998CHA
SO_2	–70.95	–296.84	1998CHA
SO_3	–94.6	–395.77	1998CHA
S_2O	–13.5	–56.48	1998CHA
HSO	–1.0	–4.2	1987LOV/WAN
HSO_2	–53	–221.8	1980BOY/GUP
$HOSO_2$	–92	385	1984MAR
SF	3.1	12.97	1998CHA
SF_2	–70.9	–296.65	1998CHA
SF_3	–120.23	–503.03	1998CHA
SF_4	–178.3 ±3.0	–763.16	1998CHA
SF_5	–210.3±4.8	–908.45	1998CHA
HSe	34.6±0.5	144.8±2.1	1994BER/ELL
HTe	37.9±1.2	156.8±5.0	1994BER/ELL
PH_2	33.1±0.6	138.5±2.5	1994BER/ELL
PH	60.6	253.55	1998CHA
AsH_2	40.1±0.3	167.8±1.3	1994BER/ELL
AsH	40.1	167.8	1988BER

(continued)

Table 11.2 (continued) Heats of Formation of Small Inorganic Radicals

Inorganic radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
SbH_2	51.5±0.6	215.5±2.5	1994BER/ELL
FO	26.0	108.78	1998CHA
ClO	24.2	101.22	1998CHA
BrO	31.9	133.5	1988LIA/BAR

11.3 Organic radicals in the gas phase

11.3.1 C-centered radicals

Table 11.3.1 Heats of Formation of C-Centered Radicals

C-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
CH	142.0	594.13	1998CHA
CH_2 (triplet)	93.3±1.0	390.4±4.2	1985BUN/SEA
CH_2 (singlet)	102.4±1.0	428.4±4.2	1985BUN/SEA
$^{\bullet}CH_3$, methyl	35.06±0.1	146.69±0.42	1987DOB/BEN
$^{\bullet}C_2H$, acetenyl, $CH{\equiv}C^{\bullet}$	135.1±0.7	565.3±2.9	1994BER/ELL
$^{\bullet}C_2H_2$, $CH_2{=}C^{\bullet\bullet}$	100.3±4	419.7±16.7	1999AHM/PET
$^{\bullet}C_2H_3$, vinyl, $CH_2{=}C^{\bullet}H$	71.6±0.8	299.6±3.3	1994BER/ELL
$^{\bullet}C_2H_5$, ethyl, $CH_3C^{\bullet}H_2$	28.4±0.3	118.8±1.3	1997DOB/BEN
$^{\bullet}C_3H_3$, propargyl, $CH{\equiv}CC^{\bullet}H_2$	81.0±1	339±4	1996TSA
$^{\bullet}C_3H_3$, $CH_3C{\equiv}C^{\bullet\bullet}$	121±3	506.3±12.6	2000SHI/ERV
$^{\bullet}C_3H_3$, $CH_2{=}C{=}CH^{\bullet} \leftrightarrow CH{\equiv}CC^{\bullet}H_2$	81.0±1	339.0±4.2	1996TSA
$^{\bullet}C_3H_3$, cyclopro-2-en-1-yl	105.1±4.1	439.7±17.2	1980DEF/MCI
$^{\bullet}C_3H_5$, allyl, $CH_2{=}CHC^{\bullet}H_2$	40.8±0.7	171±3	1996TSA
$^{\bullet}C_3H_5$, $CH_3CH{=}C^{\bullet}H$	63.8±1.5	267±6	1999TSA
$^{\bullet}C_3H_5$, $CH_3C^{\bullet}{=}CH_2$	55.3	231.4	1990TAK
$^{\bullet}C_3H_5$, cyclopropyl	66.9±2.5	279.9±10.5	1979BAG/BEN
n-C_3H_7,$^{\bullet}$ n-propyl, $CH_3CH_2C^{\bullet}H_2$	23.9±0.5	100±2	1996TSA
i-C_3H_7,$^{\bullet}$ i-propyl, $CH_3C^{\bullet}HCH_3$	21.0±0.7	88±3	1988RUS/SEE(b)
$^{\bullet}C_4H_5$, $CH_3C{\equiv}CC^{\bullet}H_2$	70.2±2	293.7±8.4	1982NGU/KIN

$^{\bullet}C_4H_5$, $CH{\equiv}CC^{\bullet}HCH_3$	70.5±2.2	295.0±9.2	1981NGU/KIN
$^{\bullet}C_4H_7$, $CH_3CH{=}CHC^{\bullet}H_2$	34.9±2.0	146±8	1999TSA
$^{\bullet}C_4H_7$, $CH_2{=}CHCH_2C^{\bullet}H_2$	46.0	192.5	1984SCH/HOU
$^{\bullet}C_4H_7$, $CH_2{=}C(CH_3)C^{\bullet}H_2$	30.6±0.6	128.0±2.5	1991ROT/BAU
$^{\bullet}C_4H_7$, $CH_2{=}CHC^{\bullet}HCH_3$	31.8±1.5	**133.1±6.5**	1987LIA/AUS
$^{\bullet}C_4H_7$, cyclopropylmethyl	51.1±1.6	213.8±6.7	1971MCM/GOL
$^{\bullet}C_4H_7$, cyclobutyl	51.4±1.0	215.1±4.2	1972MCM/GOL
n-C_4H_9,$^{\bullet}$ n-butyl, $CH_3CH_2CH_2C^{\bullet}H_2$	18.6±0.5	77.8±2.1	1990WAL/TSA
i-C_4H_9,$^{\bullet}$ i-butyl, $(CH_3)_2CHC^{\bullet}H_2$	16.7±1.0	70±4	1999TSA
s-C_4H_9,$^{\bullet}$ s-butyl, $CH_3C^{\bullet}HCH_2CH_3$	16.2±0.5	67.8±2.1	1992SEA/PIL
t-C_4H_9,$^{\bullet}$ t-butyl, $(CH_3)_3C^{\bullet}$	11.5±0.7	48±3	1996TSA
$^{\bullet}C_5H_5$, $CH_2{=}CHC{\equiv}CC^{\bullet}H_2$	84.0	351.5	1992STA/KIN
$^{\bullet}C_5H_5$, cyclopenta-1,3-dien-5-yl	63.9±2	267.4±8.4	1997ROM/JAN
$^{\bullet}C_5H_7$, $CH_3C{\equiv}CC^{\bullet}HCH_3$	65.2±2.2	272.8±9.2	1981KIN/NGU
$^{\bullet}C_5H_7$, $CH{\equiv}CC^{\bullet}HC_2H_5$	66.2±2	277.0±8.4	1976LOS/TRA
$^{\bullet}C_5H_7$, $CH{\equiv}CC^{\bullet}(CH_3)_2$	61.5±2.2	257.3±9.2	1977KIN
$^{\bullet}C_5H_7$, $CH_2{=}CHCH{=}CHC^{\bullet}H_2$	49±3	205±12.6	1982MCM/GOL
$^{\bullet}C_5H_7$, $(CH_2{=}CH)_2C^{\bullet}H$	49.7±1.0	208.0±4.2	1991CLA/CUL
$^{\bullet}C_5H_7$, $CH_3CH{=}C{=}CHC^{\bullet}H_2$	66.9	278.0	2001TUM/DEN
$^{\bullet}C_5H_7$, spiropentyl	91.0±1.0	380.7±4.2	1971FER/WHI
$^{\bullet}C_5H_7$, cyclopent-1-en-3-yl	38.4±1.0	160.7±4.2	1970FUR/GOL(b)
$^{\bullet}C_5H_9$, cyclopentyl	25.3±1.0	105.9±4.2	1982CAS/GRI
$^{\bullet}C_5H_9$, $CH_2{=}CHC^{\bullet}HCH_2CH_3$	26.2±2	109.6±8.4	1976LOS/TRA
$^{\bullet}C_5H_9$, $CH_3CH{=}CHC^{\bullet}H(CH_3)$	22	92	1988LIA/BAR
$^{\bullet}C_5H_9$, $CH_3CH{=}C(CH_3)C^{\bullet}H_2$	22.0	92.0	2001TUM/DEN
$^{\bullet}C_5H_9$, $CH_2{=}CHC^{\bullet}(CH_3)_2$	20.8±2	87.0±8.4	1970EGG/JOL
$^{\bullet}C_5H_9$, $CH_2{=}C(CH_3)C^{\bullet}H(CH_3)$	22.4	93.7	2001TUM/DEN
$^{\bullet}C_5H_9$, $CH_2{=}C(C^{\bullet}H_2)CH_2CH_3$	27.3	114.2	2001TUM/DEN
$^{\bullet}C_5H_9$, $CH_2{=}CH(CH_2)_2C^{\bullet}H_2$	42.9	179.5	1996CAM/AUT
nC_5H_{11},$^{\bullet}$ $CH_3CH_2CH_2CH_2C^{\bullet}H_2$	13	54.4	1988LIA/BAR
$^{\bullet}C_5H_{11}$, $(C_2H_5)_2C^{\bullet}H$	11.2	47.0	1996CAM/AUT
$^{\bullet}C_5H_{11}$, $(nC_3H_7)(CH_3)C^{\bullet}H$	12	50.2	1988LIA/BAR

(continued)

Table 11.3.1 (continued) Heats of Formation of C-Centered Radicals

C-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
$^{\bullet}C_5H_{11}$, $(CH_3)_3C^{\bullet}CH_2$	8.7±2	36.4±8.4	1969LAR/HAR
$^{\bullet}C_5H_{11}$, $(C_2H_5)(CH_3)_2C^{\bullet}$	7.0	29	1999TSA
$^{\bullet}C_6H_5$, phenyl	78.9±0.8	330.1±3.3	1994BER/ELL
$^{\bullet}C_6H_7$, cyclohexa-1,3-dien-5-yl	47.6	199.2	1991STE/BRO
$^{\bullet}C_6H_7$, cyclohexa-1,4-dien-3-yl	48.2±1.2	201.7±5.0	1986TSA
$^{\bullet}C_6H_9$, $CH_3C{\equiv}CC^{\bullet}(CH_3)_2$	53.0±2.2	221.8±9.2	1981KIN/NGU
$^{\bullet}C_6H_9$, $(CH_2{=}CH)_2C^{\bullet}(CH_3)$	46.3	193.7	1999LAA/MUL
$^{\bullet}C_6H_9$, cyclohexa-1-en-3-yl	28.6	119.7	1988BOR/CHE
$^{\bullet}C_6H_{11}$, $CH_2{=}CH(CH_2)_3C^{\bullet}H_2$	37.9	158.6	1996CAM/AUT
$^{\bullet}C_6H_{11}$, $CH_2{=}CHC^{\bullet}H(CH_2)_2CH_3$	21.3	89.0	2001TUM/DEN
$^{\bullet}C_6H_{11}$, $CH_2{=}C(CH_3)C^{\bullet}(CH_3)_2$	9.0±1.5	37.7±6.3	1973ROD/WU
$^{\bullet}C_6H_{11}$, $(CH_3)_2C{=}C(CH_3)C^{\bullet}H_2$	9.5±1.5	39.7±6.3	1973ROD/WU
$^{\bullet}C_6H_{11}$, $(CH_3)_2C{=}CHC^{\bullet}H(CH_3)$	11.3	47.3	2001TUM/DEN
$^{\bullet}C_6H_{11}$, (Z)-$CH_3CH{=}CHC^{\bullet}(CH_3)_2$	13.0	54.4	2001TUM/DEN
$^{\bullet}C_6H_{11}$, cyclohexyl	18±1.5	75.3±6.3	1981TSA
nC_6H_{13},$^{\bullet}$ $CH_3CH_2CH_2CH_2CH_2C^{\bullet}H_2$	8	33.5	1988LIA/BAR
$^{\bullet}C_6H_{13}$, $(nC_4H_9)(CH_3)C^{\bullet}H$	7	29.7	1988LIA/BAR
$^{\bullet}C_6H_{13}$, 2-methyl-2-pentyl	0.8±2	3.3±8.4	1983SER/GOR
$^{\bullet}C_6H_{13}$, 3-methyl-3-pentyl	3.4	14.2	1996CAM/AUT
$^{\bullet}C_6H_{13}$, 2,3-dimethyl-2-butyl	0.7±2.4	3.1±10	2000KIR/KOR
$^{\bullet}C_7H_3$, $(CH{=}C)_3C^{\bullet}$	187.5	784.5	1990TAK
$^{\bullet}C_7H_7$, benzyl, $C_6H_5C^{\bullet}H_2$	48.4±1.5	202.5 ±6.3	1994BER/ELL
$^{\bullet}C_7H_7$, quadricyclolan-5-yl	138.3 ±1.3	578.6±5.4	1996LEE/DEP
$^{\bullet}C_7H_7$, quadricyclolan-4-yl	140.4±1.3	587.4±5.4	1996LEE/DEP
$^{\bullet}C_7H_7$, norborna-2,5-dien-7-yl	122.3±1.9	511.7±7.9	1996LEE/DEP
$^{\bullet}C_7H_7$, cyclohepta-1,3,5-trien-7-yl	68.2±3	285.3±12.6	1980DEF/MCI
$^{\bullet}C_7H_9$, $(CH_2{=}CH)_3C^{\bullet}$	65.5	274.0	1990TAK
$^{\bullet}C_7H_{11}$, norborn-1-yl	32.6±2.5	136.4±10.5	1970ONE/BAG
$^{\bullet}C_7H_{11}$, cycloheptenyl	28.5	119.2	2001TUM/DEN
$^{\bullet}C_7H_{13}$, cycloheptyl	12.1±1	50.6±4.2	1971FER/WHI

$^{\bullet}C_7H_{13}$, cyclo-[$C^{\bullet}(CH_3)(CH_2)_5$]	5.4	22.6	2001TUM/DEN
$^{\bullet}C_7H_{13}$, cyclo-[$C^{\bullet}(CH_2CH_3)(CH_2)_4$]	11.2	47.0	2001TUM/DEN
$^{\bullet}C_7H_{15}$, (nC_5H_{11})$(CH_3)CH^{\bullet}$	2	8.4	1988LIA/BAR
$^{\bullet}C_8H_7$, cubyl	198.6±4	831.0±16.7	1997HAR/EMR
$^{\bullet}C_8H_9$, $C_6H_5C^{\bullet}H(CH_3)$	40.4	169.0	1982MCM/GOL
$^{\bullet}C_8H_9$, 1-phenyl-eth-2-yl	55.9	234.0	1989FRE/OLM
$^{\bullet}C_8H_9$, p-$CH_3C_6H_4C^{\bullet}H_2$	40	167.4	1986HAY/KRU
$^{\bullet}C_8H_9$, m-$CH_3C_6H_4C^{\bullet}H_2$	40	167.4	1986HAY/KRU
$^{\bullet}C_8H_9$, o-$CH_3C_6H_4C^{\bullet}H_2$	40	167.4	1986HAY/KRU
$^{\bullet}C_8H_{11}$, $C_6H_5C^{\bullet}(CH_3)_2$	32.0	134.0	1997LAA/BOR
$^{\bullet}C_8H_{13}$, CH_2=CHCH=$CHC^{\bullet}H(CH_2)_2CH_3$	31.2	130.5	2001TUM/DEN
$^{\bullet}C_8H_{13}$, CH_2=$CHC^{\bullet}H(CH_2)_3CH$=CH_2	31.2	130.5	2001TUM/DEN
$^{\bullet}C_8H_{13}$, bicyclooct-1-yl	22.0	92.0	1971DAN/TIP
$^{\bullet}C_8H_{15}$, CH_2=$CHC^{\bullet}H(CH_2)_4CH_3$	11.9	49.8	2001TUM/DEN
$^{\bullet}C_8H_{15}$, (E)-CH_3CH=$C^{\bullet}(CH_2)_4CH_3$	7.1	29.7	2001TUM/DEN
$^{\bullet}C_8H_{15}$, (Z)-$(CH_3)_2C^{\bullet}CH$=$CHCH(CH_3)_2$	2.2	9.2	2001TUM/DEN
$^{\bullet}C_8H_{15}$, cyclooctanyl	14.2	59.4	2001TUM/DEN
$^{\bullet}C_8H_{15}$, cyclo-[$C^{\bullet}(CH_2CH_3)(CH_2)_5$]	2.4	10.0	2001TUM/DEN
$^{\bullet}C_8H_{15}$, (E)-cyclo-[$C^{\bullet}(CH_3)CH(CH_3)(CH_2)_4$]	–2.1	–8.8	2001TUM/DEM
$^{\bullet}C_8H_{15}$, (Z)-cyclo-[$C^{\bullet}(CH_3)CH(CH_3)(CH_2)_4$]	1.5	6.3	2001TUM/DEM
$^{\bullet}C_9H_7$, indenyl	71	297.1	1982MCM/GOL
$^{\bullet}C_9H_9$, indanyl-1	48.8±2	204.2±8.4	2000DEN/DEN
$^{\bullet}C_9H_{11}$, 2,6-dimethylbenzyl	29.8	124.7	1980BAR/STE
$^{\bullet}C_9H_{11}$, 3,6-dimethylbenzyl	29.8	124.7	1980BAR/STE
$^{\bullet}C_9H_{11}$, 3,5-dimethylbenzyl	29.8	124.7	1980BAR/STE
$^{\bullet}C_9H_{17}$, cyclononanyl	12.5	52.3	2001TUM/DEN
$^{\bullet}C_{10}H_7$, naphth-1-yl	96.0±1.3	401.7±5.4	2000REE/KAS
$^{\bullet}C_{10}H_7$, naphth-2-yl	95.7±1.4	400.4±5.9	2000REE/KAS
$^{\bullet}C_{10}H_{11}$, tetralin-1-yl	37±1.2	154.8±5.0	1997LAA/MUL
$^{\bullet}C_{10}H_{13}$, 1-phenyl-but-4-yl	45.9	192.0	1989FRE/OLM
$^{\bullet}C_{10}H_{13}$, $(C_6H_5CH_2)(C_2H_5)C^{\bullet}H$	44.1	184.5	1989FRE/OLM
$^{\bullet}C_{10}H_{13}$, $(C_6H_5CH_2CH_2)(CH_3)C^{\bullet}H$	44.1	184.5	1989FRE/OLM

(continued)

Table 11.3.1 (continued) Heats of Formation of C-Centered Radicals

C-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
$^{\bullet}C_{10}H_{15}$, 1-adamantyl	12.3	51.5	1986KRU/BEA
$^{\bullet}C_{10}H_{15}$, 2-adamantyl	14.8	61.9	1986KRU/BEA
$^{\bullet}C_{10}H_{19}$, cyclodecanyl	7.7	32.2	2001TUM/DEN
$^{\bullet}C_{11}H_{9}$, 1-naphthylmethyl	60.4	252.7	1982MCM/GOL
$^{\bullet}C_{11}H_{21}$, cycloundecanyl	1.8	7.5	2001TUM/DEN
$^{\bullet}C_{12}H_{23}$, cyclododecanyl	–9.2	–38.5	2001TUM/DEN
$^{\bullet}C_{13}H_{9}$, 9-fluorenyl	71.1	297.5	1994RAK/VER
$^{\bullet}C_{13}H_{11}$, $(C_6H_5)_2C^{\bullet}H$	72.2±1.0	302.1±4.2	1991PAR/HAN
$^{\bullet}C_{13}H_{11}$, 9-methyl-9-fluorenyl	64.1	268.2	1994RAK/VER
$^{\bullet}C_{14}H_{11}$, 9,10-dihydroanthracen-9-yl	62.4	261.0	1991STE/BRO
$^{\bullet}C_{15}H_{11}$, 9-anthracenylmethyl	80.7	337.6	1991PAK/HAN
$^{\bullet}C_{15}H_{11}$, 9-phenanthrenylmethyl	74.4	311.3	1982MCM/GOL
$^{\bullet}C_{16}H_{31}$, $CH_2{=}CHC^{\bullet}H(CH_2)_{12}CH_3$	–28.4	–118.8	2001TUM/DEN
$^{\bullet}C_{19}H_{15}$, trityl, $(C_6H_5)_3C^{\bullet}$	93.7±2	392.0±8.4	1991PAR/HAN
$^{\bullet}C_{35}H_{25}$, pentamethylcyclopentadienyl	16.1	67.4	1995ROT/HUN
CF	57.5±2.4	240.6±10.0	1991GUR/VEY
CF_2	–44.6±1.5	–186.6±6.3	1978ROD
$FC^{\bullet}(O)$	–41	–171.5	1998CHA
CHF	34.2±3.0	143.0±12.6	1997POU/PAU
CClF	7.4±3.2	31.0±13.4	1997POU/PAU
CCl	120	502.0	1998CHA
CCl_2	54.0	226	2000BOR/ING
$ClC^{\bullet}(O)$	–5.2	–21.8	1990NIC/KRE
CHCl	78.0±2.0	326.4±8.4	1997POU/PAU
CClBr	63.8	267	2000BOR/ING
CBr	122	510.45	1998CHA
CBr_2	77.4	324	2000BOR/ING
CI	<86.8	<363.2	1977VOG/MIS
$^{\bullet}CF_3$	–111.4±0.9	–466.1±3.8	1997ASH/RUS

$^{\bullet}CHF_2$	–57.1±1	–238.9±4.2	1983PIC/ROD
$^{\bullet}CH_2F$	–7.6±1	–31.8±4.2	1983PIC/ROD
$^{\bullet}CClF_2$	–66.7±2	–279.0±8.4	1992MIY/TSC
$^{\bullet}CCl_2F$	–21.3±2	–89.0±8.4	1992MIY/TSC
$^{\bullet}CHClF$	–14.5±2.4	–60.7±10.0	1987TSC/PAD
$^{\bullet}CCl_3$	17.0±0.6	71.1±2.5	1991HUD/JON
$^{\bullet}CHCl_2$	22.3±1.0	93.3±4.2	1997POU/PAU
$^{\bullet}CH_2Cl$	28.0±0.7	117.2±2.9	1996SEE
$^{\bullet}CHBrCl$	36.8±3	154.0±13	2000BOR/ING
$^{\bullet}CHBr_2$	45.0±2.2	188.3±9.2	1987TSC/PAD
$^{\bullet}CBr_3$	49.0±2	205.0±8.4	1988HOL/LOS
$^{\bullet}CH_2Br$	40.4±1	169.0±4.2	1987TSC/PAD
$^{\bullet}CHI_2$	79.8±2.2	333.9±9.2	1970ONE/BEN
$^{\bullet}CH_2I$	54.9±2	229.7±8.4	1988HOL/LOS
$^{\bullet}C_2F$, $FC{\equiv}C^{\bullet}$	110±5	460.0±21	1996ZAR/WES
$^{\bullet}C_2F_3$, $CF_2{=}C^{\bullet}F$	–45.9±2	–192.0±8.4	1983SPY/SAU
$^{\bullet}C_2F_2H$, $CF_2{=}C^{\bullet}H$	–22.2±2	–92.9±8.4	1981STE/ROW
$^{\bullet}C_2F_2H$, $CHF{=}C^{\bullet}F$	–12.1±2	–50.6±8.4	1981STE/ROW
$^{\bullet}CCl_2H$, $CHCl{=}C^{\bullet}Cl$	56.1±2	234.7±8.4	1981STE/ROW
$^{\bullet}CClH_2$, $CH_2{=}C^{\bullet}Cl$	>60	>251.0	1989RUS/SEN
$^{\bullet}C_2F_5$, $CF_3C^{\bullet}F_2$	–213.4±1	–892.9±4.2	1981EVE/WHI
$^{\bullet}C_2HF_4$, $CF_3C^{\bullet}HF$	–162.7±2.3	–680.8±9.6	1983MAR/PAR
$^{\bullet}C_2HF_4$, $CHF_2C^{\bullet}F_2$	–158.9	–664.8	1996ZAR/WES
$^{\bullet}C_2H_2F_3$, $CF_3C^{\bullet}H_2$	–123.6±2	–517.1±8.4	1974WU/ROD
$^{\bullet}C_2H_2F_3$, $CH_2FC^{\bullet}F_2$	–107.5	–449.8	1996ZAR/WES
$^{\bullet}C_2H_2F_3$, $CHF_2C^{\bullet}HF$	–109	–456.0	1996ZAR/WES
$^{\bullet}C_2H_2F_2Cl$, $CF_2ClC^{\bullet}H_2$	–74.3±1.7	–310.9±7.0	1994PAD/CHE
$^{\bullet}C_2H_3F_2$, $CH_3C^{\bullet}F_2$	–72.3±2	–302.5±8.4	1977PIC/ROD
$^{\bullet}C_2H_3F_2$, $CHF_2C^{\bullet}H_2$	–68.3	–285.8	1996ZAR/WES
$^{\bullet}C_2H_3F_2$, $CH_2FC^{\bullet}HF$	–57.0	–238.5	1996ZAR/WES
$^{\bullet}C_2H_4F$, $CH_3C^{\bullet}HF$	–16.8±2	–70.3±8.4	1996MIY/OZA
$^{\bullet}C_2H_4F$, $CH_2FC^{\bullet}H_2$	–14.2±2	–59.4±8.4	1996MIY/OZA

(continued)

Table 11.3.1 (continued) Heats of Formation of C-Centered Radicals

C-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
$^{\bullet}C_2F_4Cl$, $CF_2ClC^{\bullet}F_2$	–164	–686	1972FOO/TAI
$^{\bullet}C_2F_3ClBr$, $CF_3C^{\bullet}ClBr$	–120.5±2	–504.2±8.4	1982MCM/GOL
$^{\bullet}C_2HF_3Cl$, $CClF_2C^{\bullet}HF$	–107.7±3	–450.6±12.6	1998SKO/DYM
$^{\bullet}C_2Cl_5$, $CCl_3C^{\bullet}Cl_2$	8.4±1.3	35.1±5.4	1969FRA/HUY
$^{\bullet}C_2HCl_4$, $CHCl_2C^{\bullet}Cl_2$	5.6±2	23.4±8.4	1976LEW
$^{\bullet}C_2H_3Cl_2$, $CH_3C^{\bullet}Cl_2$	10.2±0.4	42.5±1.7	1996SEE
$^{\bullet}C_2H_4Cl$, $CH_3C^{\bullet}HCl$	18.3±0.4	76.5±1.6	1996SEE
$^{\bullet}C_2H_4Cl$, $CH_2ClC^{\bullet}H_2$	22.2±0.6	93.0±2.4	1998SEE
$^{\bullet}C_2H_3Br_2$, $CH_3C^{\bullet}Br_2$	33.5±1.3	140.2±5.4	1999MIY/TSC
$^{\bullet}C_2H_4Br$, $BrCH_2C^{\bullet}H_2$	32.3	135.1	1988HOL/LOS
$^{\bullet}C_2H_4Br$, $CH_3C^{\bullet}HBr$	30.3	126.8	1990MIY/TSC
n-C_3F_7,$^{\bullet}$ $CF_3CF_2C^{\bullet}F_2$	104±2	435.1±8.4	1982MCM/GOL
i-C_3F_7,$^{\bullet}$ $CF_3C^{\bullet}FCF_3$	103.6±0.6	433.5±2.5	1983EVE/WEE
$^{\bullet}C_3H_6Cl$, $CH_3CH_2C^{\bullet}HCl$	13.5	56.6	1998SEE
$^{\bullet}C_6F_5$	–130.9±2	–547.7±8.4	1974KRE/PRI
$HOC^{\bullet}H_2$	–4.08±0.8	–17.07±3.35	1994BER/ELL
$HOCH_2C^{\bullet}H_2$	–7	–29.3	1990TAK
$CH_3C^{\bullet}HOH$	–13.3±0.8	–55.6±3.5	2001SUN/BOZ
$^{\bullet}C_2H_3O$, oxiran-2-yl	35.8±1.5	149.8±6.3	1984BAL/KEE
$CH_3CH_2C^{\bullet}HOH$	–19.4±1	–81±4	1999TSA
$(CH_3)C^{\bullet}HCH_2OH$	18.8±2	78.7±8.4	1992HOL
$HOCH_2CH_2C^{\bullet}H_2$	–16.0±2	–66.9±8.4	1992HOL
$(CH_3)_2C^{\bullet}OH$	–26.3±1	–110.0±4.2	1982MCM/GOL
$^{\bullet}CH_2CH(OH)CH_3$	–15.0±2.8	–62.8±11.7	2002SUN/BOZ
$^{\bullet}CH_2C(OH)(CH_3)_2$	–35.2±2	–147.3±8.4	1992HOL
$(CH_2{=}CH)_2C^{\bullet}OH$	22.1±2	92.5±8.4	1991CLA/CUL
$CH_2{=}CHC^{\bullet}HOH$	0±2	0±8.4	1973ALF/GOL
$Ph_2C^{\bullet}OH$	36.4±1.5	152.3±6.3	1973TRE
$(CH_3)_2(CH_2)C^{\bullet}OH$	–26.8±2	–121.1±8.4	1982MCM/GOL
$CH_3OC^{\bullet}H_2$	0±1	0±4.2	1999ATK/BAU

$CH_3CH_2OC^{\bullet}H_2$	–10.8±2	–45.2±8.4	1991HOL/LOS
$CH_3CH_2OC^{\bullet}HCH_3$	–19.4±1	–81.2±4.2	1986BUR/MAJ
$HOCH_2C^{\bullet}HOH$	–52.6±2	–220.1±8.4	1992HOL
$C^{\bullet}H{=}C{=}O$	41.9±2	175.3±8.4	1994BER/ELL
$HC^{\bullet}(O)$	9.96±0.20	41.67±0.84	1994BER/ELL
$CH_3C^{\bullet}(O)$	–2.4±0.2	–10.0±0.8	1994BER/ELL
$CF_3C^{\bullet}(O)$	–128.4	–537.2	1995TAK/PAS
$CH_3CH_2C^{\bullet}(O)$	–7.7±1	–32.3±4.2	2000ATK/BAU
$CH_2CHC^{\bullet}(O)$	19.3±2	80.8±8.4	1995LUN/DAA
$C_6H_5C^{\bullet}(O)$	27.8±2.6	116.3±10.9	1989SIM/GRI
$HC(O)CH_2^{\bullet}$	2.5±2.2	10.5±9.2	1994BER/ELL
$CH_3C(O)CH_2^{\bullet}$	–8.1±0.7	–34.0±3	2001BOU/CHA
$CH_3C(O)C^{\bullet}HCH_3$	–16.8±1.7	–70.3±7.1	1970SOL/BEN
$CH_3C(O)C^{\bullet}{=}CH_2$	27.1	113.4	1990TAK
$C_2H_5C(O)C^{\bullet}HCH_3$	–25.7±5	–107.5±20.9	1990BOR/HAR
$iPrC(O)C^{\bullet}(CH_3)_2$	–41.5±5	–173.6±20.9	1990BOR/HAR
$tC_4H_9C(O)C^{\bullet}H_2$	–27.6±3	–115.5±12.6	1990BOR/HAR
$PhC(O)C^{\bullet}H_2$	20.2±3	84.5±12.6	1990BOR/HAR
$PhC(O)C^{\bullet}HCH_3$	9.9±5	41.4±20.9	1990BOR/HAR
$PhC^{\bullet}HC(O)CH_2Ph$	32.1±3	134.3±20.9	1990BOR/HAR
$PhC(O)OC^{\bullet}H_2$	–16.7	–69.9	1970SOL/BEN
$^{\bullet}C(O)OH$	–46.5±0.7	–194.6±2.9	1994BER/ELL
$^{\bullet}C(O)OCH_3$	–40.5±2	–169.5±8.4	1991HOL/LOS
$C^{\bullet}H_2C(O)OH$	–60.2±2.9	–252.0±12.0	1994WEN/SQU
$C^{\bullet}H_2C(O)OCH_3$	–56.6±2	–236.8±8.4	1991HOL/LOS
$C^{\bullet}H_2C(O)OCH_2CH_3$	–62.2±3	–260.2±12.6	1995BOR/ZHA
$C^{\bullet}H_2C(O)OPh$	–6.7	–28.0	1973ALF/GOL
$^{\bullet}C_4H_7O$, tetrahydrofuran-2-yl	–4.3±1.5	–18.0±6.3	1982MCM/GOL
$^{\bullet}C_4H_8O$, cyclopentanon-2-yl	–10±3	–41.8±12.6	1991BOR/GAL
$^{\bullet}C_4H_7O_2$, 1,4-dioxan-2-yl	–31.5±3	–131.8±12.6	2000KRA/CIR
$^{\bullet}C_7H_5O_2$, 2-C(O)OH-$^{\bullet}C_6H_4$	–7.9	–33.0	1998NAS/SQU
$^{\bullet}C_7H_5O_2$, 3-C(O)OH-$^{\bullet}C_6H_4$	–8.4	–35.0	1998NAS/SQU

(continued)

Table 11.3.1 (continued) Heats of Formation of C-Centered Radicals

C-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
$^{\bullet}C_7H_5O_2$, 4-C(O)OH-$^{\bullet}C_6H_4$	–8.6	–36.0	1998NAS/SQU
$^{\bullet}CHN_2$	118.2	494.5	1996FUL/HIP
$^{\bullet}CH_2NH_2$	36.3±2	151.9±8.4	1983BUR/CAS
$CH_3C^{\bullet}HNH_2$	26.7±2	111.7±8.4	1983BUR/CAS
$(CH_3)_2C^{\bullet}NH_2$	16.7±2	69.9±8.4	1983BUR/CAS
$^{\bullet}CH_2NHCH_3$	30.5±2	127.6±8.4	1981GRI/LOS
$^{\bullet}CH_2N(CH_3)_2$	33.2±2	139.0±8.4	1999LAA/MUL
$(C_2H_5)_2NC^{\bullet}HCH_3$	16.4±0.5	68.6±2.1	1990DOM/DIN
$^{\bullet}CH_2N(CH_3)Ph$	63.6±3	266.0±12.6	1999DOM/DIN
$^{\bullet}CH_2NC$	78.0±2.7	326.4±11.3	1987MOR/ELL(b)
$^{\bullet}CN$	105.5±1.1	441.4±4.6	1994BER/ELL
$^{\bullet}CH_2CN$	60.4±1	252.6±4	2000LAF/SZA
$CH_3C^{\bullet}HCN$	54.2±3	226.7±12.6	1999SEN/IKE
$(CH_3)_2C^{\bullet}CN$	45.5±3	190.4±12.6	1998BRO/BEC
$Ph(CH_3)C^{\bullet}CN$	59.4±2	248.5±8.4	1982MEO
$H_2C^{\bullet}NN$	69.9±0.5	292.5±2.1	2000BIS/HOO
$^{\bullet}CH_2NO_2$	27.5±3	115.1±12.6	1994BOR/SAT
$CH_3C^{\bullet}HNO_2$	14.8±3	61.9±12.6	1994BOR/SAT
$(CH_3)_2C^{\bullet}NO_2$	1.5±3	6.3±12.6	1994BOR/SAT
$PhC^{\bullet}HNO_2$	40.4±3	169.0±12.6	1995BOR/ZHA(c)
$^{\bullet}C_6H_6N$, 3-NH_2-C_6H_4	76.5	320.1	1975MAT/NAS
$^{\bullet}C_6H_4NO_2$, 3-NO_2-C_6H_4	81.4±2.4	340.6±10.0	1985GON/LAR
$^{\bullet}C_6H_3N_2O_4$, 3,5-$(NO_2)_2$-C_6H_3	73.0	305.4	1975MAT/NAS
$^{\bullet}C_7H_6NO_2$, 2-Me-4-NO_2-C_6H_3	70.6±2	295.4±8.4	1985GON/LAR
$^{\bullet}C_4H_3N$, pyrrol-2-yl	92.2	385.8	1991MAC/COL
$^{\bullet}C_4H_3N$, pyrrol-3-yl	92.2	385.8	1991MAC/COL
$^{\bullet}C_4H_8N$, pyrrolidin-2-yl	34.1±3	142.7±12.6	2000KRA/CIR
$^{\bullet}C_5H_4N$, pyrid-2-yl	86.5	362.0	1997KIE/ZHA
$^{\bullet}C_5H_4N$, pyrid-3-yl	93.5	391.0	1997KIE/ZHA
$^{\bullet}C_5H_4N$, pyrid-4-yl	93.5	391.0	1997KIE/ZHA

$^{\bullet}C_4H_7N_2$, piperad-2-yl	28.6	119.7	1997WAY/CLA
$^{\bullet}C_4H_3N_2$, pyrimid-2-yl	92.7	388.0	1997KIE/ZHA
$^{\bullet}C_4H_3N_2$, pyrimid-4-yl	97.7	409.0	1997KIE/ZHA
$^{\bullet}C_4H_3N_2$, pyrimid-5-yl	106.7	446.4	1997KIE/ZHA
CS	55.9	233.9	2002CRC
C$^{\bullet}$(S)H	71.8±2	300.4±8.4	1994BER/ELL
$^{\bullet}CH_2SH$	36.3±2	151.9±8.4	1994BER/ELL
$^{\bullet}CH_2SCH_3$	32.7±1.4	136.8±5.9	1994JEF/NIC
$^{\bullet}CH_2SPh$	64.2±3	268.6±12.6	1993ZHA/BOR
$^{\bullet}CH_2SOCH_3$	5.7±3	23.8±12.6	1998BOR/LIU
HOC$^{\bullet}$(S)S	26.4	110.5	1990MUR/LOV
$^{\bullet}CH_2SO_2CH_3$	–42.3±3	–177.0±12.6	1992BOR/HAR
$^{\bullet}CH_2SO_2Ph$	–13.7±3	–57.3±12.6	1992BOR/HAR
PhC$^{\bullet}$HSO$_2$CH$_3$	–26.1±3	–109.2±12.6	1992ZHA/BOR
PhC$^{\bullet}$HSO$_2$Ph	1.7±3	7.0±12.6	2001ORL/TUR
Ph$_2$C$^{\bullet}$SO$_2$Ph	24.4±3	102.0±12.6	2001ORL/TUR
Ph$_2$C$^{\bullet}$SPh	104.1±3	435.6±12.6	2001ORL/TUR
NC$^{\bullet}$(O)	30.4	127.2	1996ZYR/DRO
$^{\bullet}CNO$	97.3	407.1	1987KOC/FRE
$^{\bullet}CH_2SiMe_3$	–7.6±1.5	–32±6	1998BEC/WAL
$^{\bullet}CH_2C(CH_3)_2SiMe_3$	–29.8	–125	1998BEC/WAL

11.3.2 O–centered radicals

Table 11.3.2 Heats of Formation of O-Centered Radicals

	$\Delta_f H°(R)$		
O-centered radicals	kcal/mol	kJ/mol	References
HO$^{\bullet}$	9.40±0.05	39.33±0.21	1994BER/ELL
FO$^{\bullet}$	26	108.8	1998CHA
ClO$^{\bullet}$	24.2	101.3	1998CHA
BrO$^{\bullet}$	30	125.5	1998CHA
IO$^{\bullet}$	30	125.5	1998CHA
HOO$^{\bullet}$	3.5	14.6	1983SHU/BEN

(continued)

Table 11.3.2 (continued) Heats of Formation of O-Centered Radicals

O-centered radicals	$\Delta_f H°(R)$ kcal/mol	$\Delta_f H°(R)$ kJ/mol	References
$FOO^{\bullet}$	6.2	25.9	1987PAG/RAT
$ClOO^{\bullet}$	23.3	97.5	1991NIC/KRE
$OClO^{\bullet}$	22.8	95.4	1994NIC/FRI
$NCO^{\bullet}$	44.0	184.1	1990TAK
sym-ClO_3	51.9±5	217.2±21	1992COL/SAN
$HSOO^{\bullet}$	26.8	112.0	1999ARM
$CH_3SOO^{\bullet}$	18.2	760	1999ARM
$CF_3SO_2O^{\bullet}$	–218	–912.0	1995TAK/PAS
O_3	34.1	142.7	1998CHA
$NCO^{\bullet}$	44.0	184.0	1990TAK
$O_2NO^{\bullet}$	15.4	64.4	1988MCD/DAV
$CH_3O^{\bullet}$	4.1±0.9	17.2±3.8	1994BER/ELL
CH_2=CH-$O^{\bullet}$	4.4±0.3	18.4±1.3	2002SEB/BOC
$C_2H_5O^{\bullet}$	–3.7±0.8	–15.5±3.3	1994BER/ELL
$nC_3H_7O^{\bullet}$	–7.2±2	–30.1±8.4	1973BEN/ONE
$iC_3H_7O^{\bullet}$	–12.5	52.3	1974BAT/CHR
$nC_4H_9O^{\bullet}$	–15	62.8	1974BAT/CHR
$sC_4H_9O^{\bullet}$	–16.6	–69.5	1974BAT/CHR
$tC_4H_9O^{\bullet}$	–22.3	–93.3	1997BEN/COH
$C_6H_5O^{\bullet}$	12.9±1.5	54±6	1996TSA
$C_6H_5CH_2O^{\bullet}$	25.6±3	107.1±12.6	1996BOR/LIU
$C_{10}H_7O,^{\bullet}$ naphthoxy-1	39.5	165.3	1975MAH/DAR
$C_{10}H_7O,^{\bullet}$ naphthoxy-2	41.6	174.1	1975MAH/DAR
$CF_3O^{\bullet}$	–151.8±1.7	–635.1±7.1	2000REI/PRA
$HC(O)O^{\bullet}$	–36.0±2	–150.6±8.4	1976BEN
$FC(O)O^{\bullet}$	–88	368.0	1995TAK/PAS
$CH_3C(O)O^{\bullet}$	–49.6 ±1	–207.5±4.2	1973BEN/ONE
$CF_3C(O)O^{\bullet}$	–190.5	–797.0	1995TAK/PAS
$CH_3CH_2C(O)O^{\bullet}$	–54.6±1	–228.4±4.2	1973BEN/ONE
$nC_3H_7C(O)O^{\bullet}$	–59.6±1	–249.4±4.2	1973BEN/ONE

$C_6H_5C(O)O^{\bullet}$	–17.4±2	–72.8±8.4	1994BOR/SAT
$CH_3OO^{\bullet}$	2.2±1.2	9.0±5.1	1998KNY/SLA(b)
$C_2H_5OO^{\bullet}$	–6.5±2.4	–27.4±9.9	1998KNY/SLA(b)
$iC_3H_7OO^{\bullet}$	–15.6±2.7	–65.4±11.3	1998KNY/SLA(b)
$tC_4H_9OO^{\bullet}$	–24.3±2.2	–101.5±9.2	1998KNY/SLA(b)
$CH_2=CHCH_2OO^{\bullet}$	21.2	88.7	2002LEE/CHE
$CH_3CH=CHCH_2OO^{\bullet}$	19.7±1.3	82.6±5.3	1998KNY/SLA
$C_6H_5CH_2OO^{\bullet}$	27.4±1	114.6±4.2	1993ELM/MIN
c-$C_6H_7OO^{\bullet}$ R=cyclohexadienyl	36.2±3	151.6±12.6	2000KRA/CIR
c-$C_6H_{11}OO^{\bullet}$	–6.0±2.5	–25.0±10.5	2000KRA/CIR
c-$C_4H_8NOO^{\bullet}$ R=pyrrolidin-2-yl	24.2±3	101.3±12.6	2000KRA/CIR
$(C_2H_5)N(CH_3)CHOO^{\bullet}$	–8.6±3	–36.0±12.6	2000KRA/CIR
C_4H_7O-$OO^{\bullet}$ R=tetrahydrofuran-2-yl	–36.3±4	–152.0±16.7	2000KRA/CIR
$C_4H_7O_2$-$OO^{\bullet}$ R=dioxan-2-yl	–65.5±4	–274.0±16.7	2000KRA/CIR
$HOCH_2OO^{\bullet}$	–38.7±0.5	–162.0±2.0	1992LIG/COX
$CH_3C(O)OO^{\bullet}$	–41.1±4.8	–172.0±20.0	1991BRI/CAR
$CF_3OO^{\bullet}$	–146.7±3.7	–614.0±15.4	1992LIG/COX
$CF_2ClOO^{\bullet}$	–97.2±3.5	–406.7±14.6	1992LIG/COX
$CFCl_2OO^{\bullet}$	–51.1	–213.8	1992LIG/COX
$CH_2ClOO^{\bullet}$	–1.2±3.3	–5.1±13.6	1998KNY/SLA(b)
$CHCl_2OO^{\bullet}$	–4.6±2.7	–19.2±11.2	1998KNY/SLA(b)
$CCl_3OO^{\bullet}$	–5.0±2.1	–20.9±8.9	1998KNY/SLA(b)
$CH_3CHClOO^{\bullet}$	–13.1±0.8	–54.7±3.4	1998KNY/SLA(b)
$CH_3CCl_2OO^{\bullet}$	–15.2±2.3	–63.8±9.8	1998KNY/SLA(b)

11.3.3 N-centered radicals

Table 11.3.3 Heats of Formation of N-Centered Radicals

	$\Delta_f H^o(R)$		
N-centered radicals	kcal/mol	kJ/mol	References
ON	21.58	90.29	1998CHA
NO_2	7.91	33.10	1998CHA
ONOO	17.0	71.1	1998CHA

(continued)

Table 11.3.3 (continued) Heats of Formation of N-Centered Radicals

N-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
N_2O	19.61	82.05	1998CHA
NH	90.0	376.6	1998CHA
$^{\bullet}NH_2$	45.1±0.3	188.7±1.3	1994BER/ELL
$HON^{\bullet}$	27.0	113.0	1996DIX
$^{\bullet}N_3$	112±5	486.6±20.9	1982MCM/GOL
$^{\bullet}N_2H_3$	58.2	243.5	1988GRE/COL
(Z)-N_2H_2	50.9	213	1998CHA
NF	50	209.2	1979HUB/HER
$^{\bullet}NF_2$	10.1	42.3	1998CHA
FNO	–15.7	–65.7	1998CHA
ClNO	12.36	51.71	1998CHA
BrNO	19.63	82.13	1998CHA
INO	26.8	112.1	1998CHA
NCO	31.3	131	1999ARM(b)
$NH_2C(O)N^{\bullet}H$	0.2±3	0.8±12.6	1991BOR/JI(b)
$CH_3C(O)N^{\bullet}H$	–1.6±3	–6.7±12.6	1991BOR/JI(b)
$NH_2C(S)N^{\bullet}H$	46.4±3	194.0±12.6	2001ORL/TUR
$CH_3C(S)N^{\bullet}H$	41.3±3	173.0±12.6	2001ORL/TUR
$PhC(S)N^{\bullet}H$	73.4±3	307.0±12.6	2001ORL/TUR
$HCON^{\bullet}H$	11.9±3	49.8±12.6	1995BOR/ZHA
$NH_2C(NH)N^{\bullet}H$	59.9±3	250.6±12.6	1991BOR/JI(b)
$^{\bullet}NHCN$	79.4	332.2	1993ESP/COR
$NCN^{\bullet}$	111.1±0.7	464.8±3	1999BIS/CHO
$HN^{\bullet}CN$	76.3±0.7	319.2±3	2001BIS/HOO
$CH_2N^{\bullet}H$	25.0±3	104.6±12.6	1988GRE/COL
$CH_3N^{\bullet}H$	44.0±2	184.1±8.4	1988COL
$tBuN^{\bullet}H$	22.8±3	95.4±12.6	1998BOR/LIU
$C_6H_5CH_2N^{\bullet}H$	68.9±3	288.3±12.6	1998BOR/LIU
$C_6H_5N^{\bullet}H$	58.4±1	244.3±4.2	1997MAC/WAY

$(CH_3)_2N^{\bullet}$	37.8±2	158.2±4.2	1988COL
$(C_6H_5)(CH_3)N^{\bullet}$	57.6±1	241.0±6.3	1993BOR/ZHA
$(C_6H_5)_2N^{\bullet}$	87.5±1.5	366.0±6.3	1997MAC/WAY
1-pyrrolyl	70.8±3	269.2±12.6	1991BOR/JI(b)
carbazol-9-yl	91.6±2	383.3±4.2	1992ARE/VEN
$CH_3N_2^{\bullet}$	51.5±1.8	215.5±7.5	1987ACS/PET
$C_2H_5N_2^{\bullet}$	44.8±2.5	187.4±10.5	1987ACS/PET
$iC_3H_7N_2^{\bullet}$	34.9±2	146.0±8.4	this volume
$nC_4H_9N_2^{\bullet}$	33.6±2	140.6±8.4	this volume
$tC_4H_9N_2^{\bullet}$	23.3±2	97.5±4.2	this volume

11.3.4 S-centered radicals

Table 11.3.4 Heats of Formation of S-Centered Radicals

	$\Delta_f H^o(R)$		
S-centered radicals	kcal/mol	kJ/mol	References
SO	1.2	5.0	1998CHA
SO_2	–70.95	–296.84	1998CHA
SO_3	–94.6	–395.8	1998CHA
S_2O	–13.5	–56.5	1998CHA
$HOS^{\bullet}$	–0.9±0.7	–3.8±2.9	1993BAL/CAS
$HC(O)S^{\bullet}$	13.5	56.5	1990TAK
$HS^{\bullet}O_2$	–53	–221.8	1980BOY/GUP
$HOS^{\bullet}O_2$	–92	–384.9	1984MAR
$NCS^{\bullet}$	71.7±2	300.0±8.0	1999ARM
$HS^{\bullet}$	34.18±0.68	143.01±2.85	1994BER/ELL
$CH_3S^{\bullet}$	29.8±0.4	124.7±1.7	1994BER/ELL
$C_2H_5S^{\bullet}$	24.1	101	1999ARM
$nC_3H_7S^{\bullet}$	19.1	80	1999ARM
$C_6H_5S^{\bullet}$	58.0±1.1	242.7±4.6	2002SAN/MUR
$C_6H_5CH_2S^{\bullet}$	58.9	246.0	2001ORL/TUR
$CH_3S^{\bullet}O_2$	–57.2	–239.3	1971SOL/BEN
$HSS^{\bullet}$	27.6±3.5	115.5±14.6	1993OHA/DEP

(continued)

Table 11.3.4 (continued) Heats of Formation of S-Centered Radicals

S-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
$CH_3SS^\bullet$	16.4±2	68.6±8.4	1986HOW/GRI
$C_2H_5SS^\bullet$	10.4±2	43.5±8.4	1986HOW/GRI
$iC_3H_7SS^\bullet$	3.3±2	13.8±8.4	1986HOW/GRI
$tC_4H_9SS^\bullet$	–4.6±2	–19.2±8.4	1986HOW/GRI
$HOC(S)S^\bullet$	26.4	110.5	1990MUR/LOV
$HC(O)S^\bullet$	13.5	56.5	1990TAK
SF	3.1	13.0	1998CHA
SF_2	–70.9	–296.7	1998CHA
SF_3	–120.2	–503.0	1998CHA
SF_4	–178.3±3	–746.0±12.6	1998CHA
SF_5	–210.3±4.8	–879.9±21	1998CHA
SN	63.0	263.6	1998CHA

11.3.5 Si, Ge-, and Sn-centered radicals

Table 11.3.5 Heats of Formation of Si, Ge-, and Sn-Centered Radicals

Si, Ge-, Sn-centered radicals	$\Delta_f H^o(R)$ kcal/mol	$\Delta_f H^o(R)$ kJ/mol	References
SiF	–4.8	–20.1	1998CHA
SiF_2	–152.5±1.5	–638±6	1998BEC/WAL
$^\bullet SiF_3$	–235.9±4	–987±20	1998BEC/WAL
SiCl	47.4	199.6	1998CHA
$SiCl_2$	–40.4±0.7	–169±3	1998BEC/WAL
$^\bullet SiCl_3$	–77.0±2	322±8	1998BEC/WAL
SiBr	56.2	235.1	1988CHA
$SiBr_2$	–11.0±2	46±8	1998BEC/WAL
$^\bullet SiBr_3$	–48.2	–201.7	1998CHA
SiI	75.0	313.8	1998CHA
SiI_2	22.0±2	92±8	1998BEC/WAL
$^\bullet SiI_3$	8.4	35.1	1998CHA

SiH	90	376.6	1998CHA
SiH_2	65.2±0.5	273±2	1998BEC/WAL
$^{\bullet}SiH_3$	47.9±0.6	200.4±2.5	1994BER/ELL
$MeSi^{\bullet}H_2$	33.7±1.5	141±6	1998BEC/WAL
$Me_2Si^{\bullet}H$	18.6±1.5	78±6	1998BEC/WAL
$Me_3Si^{\bullet}$	3.6±1.6	15±7	1998BEC/WAL
$H_3SiSi^{\bullet}H_2$	55.9±1.5	234±6	1998BEC/WAL
$C_6H_5Si^{\bullet}H_2$	65.5	274	1998BEC/WAL
$H_3SiSi^{\bullet}H$	74.6±2	312±8	1998BEC/WAL
$MeSi^{\bullet}H$	48.3±1.5	202±6	1998BEC/WAL
$Me_2Si^{\bullet\bullet}$	32.3±2	135±8	1998BEC/WAL
$^{\bullet}GeH_3$	53.0±2	221.8±8.4	1994BER/ELL

11.4 Group additivity values for organic radicals

The group additivity values (GAVs) are available in 1976BEN, and updated GAVs are available in 1993COH/BEN, 1996COH, and 1997BEN/COH.

Table 11.4.1 GAVs of C/H Radicals

	GAVs		
C/H radical groups	kcal/mol	kJ/mol	References
$^{\bullet}C\text{-}(C)(H)_2$	38.4	160.7	1999COH
$^{\bullet}C\text{-}(C)_2(H)$	41.0	171.5	1999COH
$^{\bullet}C\text{-}(C)_3$	41.6	174.1	this volume
$^{\bullet}C\text{-}(C_d)(H)_2$	25.9	108.4	this volume
$^{\bullet}C\text{-}(C_d)_2(H)$	18.5	77.4	this volume
$^{\bullet}C\text{-}(C)(C_d)(H)$	26.2	109.6	this volume
$^{\bullet}C\text{-}(C)_2(C_d)$	26.0	108.8	this volume
$^{\bullet}C\text{-}(C)(C_d)_2$	25.0	104.6	this volume
$^{\bullet}C\text{-}(C_B)(H)_2$	26.5	110.9	this volume
$^{\bullet}C\text{-}(C)(C_B)(H)$	28.5	119.2	this volume
$^{\bullet}C\text{-}(C)_2(C_B)$	30.1	125.9	this volume
$^{\bullet}C\text{-}(C_B)_2(H)$	28.3	118.4	this volume
$^{\bullet}C\text{-}(C_B)_2(C)$	30.1	125.9	this volume

(continued)

Table 11.4.1 (continued) GAVs of C/H Radicals

C/H radical groups	GAVs kcal/mol	GAVs kJ/mol	References
$^{\bullet}C\text{-}(C_B)_3$	28.9	120.9	this volume
$^{\bullet}C\text{-}(C_t)(H)_2$	26.1	109.2	this volume
$^{\bullet}C\text{-}(C)(C_t)(H)$	28.5	119.2	this volume
$^{\bullet}C\text{-}(C)_2(C_t)$	27.8	116.3	this volume
$^{\bullet}C_B\text{-}$	62.5	261.5	this volume
$^{\bullet}C_d\text{-}(H)$	65.3	273.2	this volume
$^{\bullet}C_t\text{-}$	108.0	451.9	this volume
$C\text{-}(^{\bullet}C)(H)_3$	–10.0	–41.8	1999COH
$C\text{-}(C)(^{\bullet}C)(H)_2$	–5.0	–20.9	1999COH
$C\text{-}(C)_2(^{\bullet}C)(H)$	–2.4	–10.0	1999COH
$C\text{-}(C)_3(^{\bullet}C)$	0.5	2.1	1999COH
$C_d\text{-}(^{\bullet}C)(H)$	8.6	36.0	1999COH
$C_d\text{-}(^{\bullet}C)(C)$	10.2	42.7	1999COH
$C_t\text{-}(^{\bullet}C)$	27.3	114.2	1999COH
$C_B\text{-}(^{\bullet}C)$	5.5	23.0	1999COH

Table 11.4.2 GAVs of O/C/H Radicals

O/C/H radical groups	GAVs kcal/mol	GAVs kJ/mol	References
$^{\bullet}C\text{-}(O)(H)_2$	33.5	140.2	this volume
$^{\bullet}C\text{-}(C)(O)(H)$	35.0	146.4	this volume
$^{\bullet}C\text{-}(C)_2(O)$	31.6	132.2	this volume
$^{\bullet}C\text{-}(C_d)(O)(H)$	23.0	96.2	1999COH
$^{\bullet}C\text{-}(C_d)_2(O)$	30.4	127.2	this volume
$^{\bullet}C\text{-}(C_B)_2(O)$	30.4	127.2	this volume
$^{\bullet}C\text{-}(CO)(H)_2$	32.8	137.2	this volume
$^{\bullet}C\text{-}(C)(CO)(H)$	32.6	136.4	this volume
$^{\bullet}O\text{-}(C)$	14.6	61.1	this volume
$^{\bullet}O\text{-}(C_d)$	–10.8	–45.2	this volume
$^{\bullet}O\text{-}(C_B)$	–2.7	–11.3	this volume

•O-(CO)	4.2	17.6	this volume
•O-(O)	16.4	68.6	this volume
•CO-(H)	10	41.8	this volume
•CO-(C)	7.6	31.8	this volume
•CO-(C_d)	8.0	33.5	this volume
•CO-(C_B)	5.9	24.7	1999COH
•CO-(O)	12.0	50.2	this volume
C-(•O)$(H)_3$	–10.0	–41.8	1999COH
C-(C)(•O)$(H)_2$	–8.1	–33.9	1993COH/BEN
C-(•C)(O)$(H)_2$	–8.1	–33.9	1993COH/BEN
C-$(C)_2$(•O)(H)	–7.2	–30.1	1993COH/BEN
C-(C)(•C)(O)(H)	–7.2	–30.1	1993COH/BEN
C-$(C)_3$(•O)	–6.6	–27.6	1993COH/BEN
C-$(C)_2$(•C)(O)	–6.6	–27.6	1993COH/BEN
C_B-(•O)	–0.9	–3.8	1993COH/BEN
C_d-(•O)(H)	8.6	36.0	1993COH/BEN
C_d-(•CO)(H)	5.0	20.9	1993COH/BEN
C-(•CO)$(H)_3$	–10.0	–41.8	1999COH
C-(C)(•CO)$(H)_2$	–5.2	–21.8	1993COH/BEN
C_B-(•CO)	3.7	15.5	1993COH/BEN
O-(•C)(H)	–37.9	–158.6	1999COH
O-(•C)(C)	–23.5	–98.3	1993COH/BEN
O-(•O)(C)	–4.5	–18.8	1993COH/BEN
O-(•CO)(H)	–58.0	–242.7	1993COH/BEN
O-(•CO)(C)	–43.1	–180.3	1993COH/BEN
O-(•C)(CO)	–43.1	–180.3	1993COH/BEN
O-(O)(•O)	19.0	79.5	1993COH/BEN
O-(CO)(•O)	–19.0	–79.5	1993COH/BEN
O-(C_B)(•O)	–4.6	–19.2	this volume
CO-(•C)(H)	–29.4	–123.0	1993COH/BEN
CO-(•C)(C)	–31.7	–132.6	1993COH/BEN
CO-(C)(•O)	–35.2	–147.3	1993COH/BEN
CO-(H)(•O)	–32.1	–134.3	1993COH/BEN

Table 11.4.3 GAVs of N/C/H/O Radicals

N/C/H/O radical groups	GAVs kcal/mol	GAVs kJ/mol	References
•N-$(C)_2$	57.8	241.8	this volume
•N-(C)(H)	54.0	225.9	1999COH
•N-(N)(H)	46.8	195.8	1999COH
•N-(C_B)(H)	42.5	177.8	this volume
•N-(C)(C_B)	51.7	216.3	this volume
C-(•N)$(H)_3$	–10.0	–41.8	1999COH
C_B-(•N)	–0.5	–2.1	1999COH
N-(•N)$(H)_2$	11.4	47.7	1976BEN
N-(•C)$(H)_2$	4.8	20.1	1976BEN
N-(•C)(C)(H)	9.0	37.7	1999COH
N-(•C)$(C)_2$	24.4	102.1	1976BEN
N-(•C)(C)(C_B)	26.2	109.6	1976BEN
•C-(N)$(H)_2$	31.5	131.8	this volume
•C-(C)(N)(H)	33.6	140.6	this volume
•C-$(C)_2$(N)	31.9	133.5	this volume
•C-(CN)$(H)_2$	60.4	252.6	this volume
•C-(C)(CN)(H)	64.2	268.6	this volume
•C-$(C)_2$(CN)	65.5	274.1	this volume
•C-(C)(C_B)(CN)	44.4	185.8	1999COH
(CN)-(•C)	3.0	12.6	1999COH
(•NN)-(C)	61.5	257.3	1999COH
C-(•NN)$(H)_3$	–10.0	–41.8	1999COH
C-(C)(•NN)$(H)_2$	–6.7	–28.0	1999COH
C-$(C)_2$(•NN)(H)	–6.6	–27.6	this volume
C-$(C)_3$(•NN)	–8.2	–34.3	this volume
NO_2-(•C)	–9.3	–38.9	this volume
•C-$(NO_2)(H)_2$	36.6	153.1	this volume
•C-(NO_2)(C)(H)	34.1	142.7	this volume
•C-$(NO_2)(C)_2$	30.8	128.9	this volume
•C-$(NO_2)(C_B)$(H)	27.8	116.3	this volume

Table 11.4.4 GAVs of S/C/H/O Radicals

S/C/H/O radical groups	GAVs kcal/mol	GAVs kJ/mol	References
•S-(C)	39.5	165.3	this volume
•S-(C_B)	41.6	174.1	this volume
•SO_2-(C)	–47.2	–197.5	this volume
•S-(S)	19.4	81.2	this volume
S-(•S)(H)	8.2	34.3	this volume
S-(•S)(C)	6.72	28.15	1993COH/BEN
S-(•C)(H)	4.68	19.58	1993COH/BEN
S-(•C)(C)	11.34	47.45	1993COH/BEN
S-(•C)(C_B)	16.2	68.2	1993COH/BEN
SO-(•C)(C)	–14.4	–60.2	1976BEN
SO_2-(•C)(C)	–69.7	–291.6	1976BEN
SO_2-(•C)(C_B)	–72.3	–302.5	1976BEN
•C-(S)(H)	71.8	300.4	this volume
•C-(S)$(H)_2$	31.5	131.8	this volume
•C-(SO)$(H)_2$	30.1	125.9	this volume
•C-(SO_2)$(H)_2$	38.6	161.5	this volume
•C-(SO_2)(C_B)(H)	33.8	141.4	this volume
•C-(SO_2)$(C_B)_2$	34.1	142.7	this volume
•C-(S)$(C_B)_2$	28.5	119.2	this volume

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