APPENDIX A

USEFUL TABLES AND CHARTS

# USEFUL PROPERTY DATA FOR CORRESPONDING STATES ESTIMATES

The values given in Table A.1 are useful in “corresponding

states” estimates of thermodynamic properties.

Bar ¼ 0.987 atm.

Table A.1 Property Data for Corresponding States Estimates

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Molar Mass  (¼ Molecular Weight) *M* (g/mol) | v | *Tc*(K) | *Pc* (bar) | *zc* |
| Methane | 16.043 | 0.012 | 190.6 | 45.99 | 0.286 |
| Ethane | 30.07 | 0.1 | 305.3 | 48.72 | 0.279 |
| Propane | 44.097 | 0.152 | 369.8 | 42.48 | 0.276 |
| *n*-Butane | 58.123 | 0.2 | 425.1 | 37.96 | 0.274 |
| *n*-Pentane | 72.15 | 0.252 | 469.7 | 33.7 | 0.27 |
| *n*-Hexane | 86.177 | 0.301 | 507.6 | 30.25 | 0.266 |
| *n*-Heptane | 100.204 | 0.35 | 540.2 | 27.4 | 0.261 |
| *n*-Octane | 114.231 | 0.4 | 568.7 | 24.9 | 0.256 |
| *n*-Nonane | 128.258 | 0.444 | 594.6 | 22.9 | 0.252 |
| *n*-Decane | 142.285 | 0.492 | 617.7 | 21.1 | 0.247 |
| Isobutane | 58.123 | 0.181 | 408.1 | 36.48 | 0.282 |
| Isooctane | 114.231 | 0.302 | 544 | 25.68 | 0.266 |
| Cyclopentane | 70.134 | 0.196 | 511.8 | 45.02 | 0.273 |
| Cyclohexane | 84.161 | 0.21 | 533.6 | 40.73 | 0.273 |
| Methylcyclopentane | 84.161 | 0.23 | 532.8 | 37.85 | 0.272 |
| Methylcyclohexane | 98.188 | 0.235 | 572.2 | 34.71 | 0.269 |
| Ethylene | 28.054 | 0.087 | 282.3 | 50.4 | 0.281 |
| Propylene | 42.081 | 0.14 | 365.6 | 46.65 | 0.289 |
| 1-Butene | 56.108 | 0.191 | 420 | 40.43 | 0.277 |
| *cis*-2-Butene | 56.108 | 0.205 | 435.6 | 42.43 | 0.273 |
| *trans*-2-Butene | 56.108 | 0.218 | 428.6 | 41 | 0.275 |
| 1-Hexene | 84.161 | 0.28 | 504 | 31.4 | 0.265 |
| Isobutylene | 56.108 | 0.194 | 417.9 | 40 | 0.275 |
| 1,3-Butadiene | 54.092 | 0.19 | 425.2 | 42.77 | 0.267 |
| Cyclohexene | 82.145 | 0.212 | 560.4 | 43.5 | 0.272 |

(*continued* )

*Physical and Chemical Equilibrium for Chemical Engineers*, Second Edition. Noel de Nevers.

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303

304 APPENDIX A: USEFUL TABLES AND CHARTS

Table A.1 (*Continued*)

Molar Mass

(¼ Molecular Weight) *M* (g/mol) v *Tc*(K) *Pc* (bar) *zc*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Acetylene | 26.038 | 0.187 | 308.3 | 61.39 | 0.271 |
| Benzene | 78.114 | 0.21 | 562.2 | 48.98 | 0.271 |
| Toluene | 92.141 | 0.262 | 591.8 | 41.06 | 0.264 |
| Ethylbenzene | 106.167 | 0.303 | 617.2 | 36.06 | 0.263 |
| Cumene | 120.194 | 0.326 | 631.1 | 32.09 | 0.261 |
| *o*-Xylene | 106.167 | 0.31 | 630.3 | 37.34 | 0.263 |
| *m*-Xylene | 160.167 | 0.326 | 617.1 | 35.36 | 0.259 |
| *p*-Xylene | 160.167 | 0.322 | 616.2 | 35.11 | 0.26 |
| Styrene | 104.152 | 0.297 | 636 | 38.4 | 0.256 |
| Naphthalene | 128.174 | 0.302 | 748.4 | 40.51 | 0.269 |
| Biphenyl | 154.211 | 0.365 | 789.3 | 38.5 | 0.295 |
| Formadlehyde | 30.026 | 0.282 | 408 | 65.9 | 0.223 |
| Acetaldehyde | 44.053 | 0.291 | 466 | 55.5 | 0.221 |
| Methyl acetate | 74.079 | 0.331 | 506.6 | 47.5 | 0.257 |
| Ethyl acetate | 88.106 | 0.366 | 523.3 | 38.8 | 0.255 |
| Acetone | 58.08 | 0.307 | 508.2 | 47.01 | 0.233 |
| Methyl ethyl ketone | 72.107 | 0.323 | 535.5 | 41.5 | 0.249 |
| Diethyl ether | 74.123 | 0.281 | 466.7 | 36.4 | 0.263 |
| Methyl *tert-*butyl ether | 88.15 | 0.266 | 497.1 | 34.3 | 0.273 |
| Methanol | 32.042 | 0.564 | 512.6 | 80.97 | 0.224 |
| Ethanol | 46.069 | 0.645 | 513.9 | 61.48 | 0.24 |
| 1-Propanol | 60.096 | 0.622 | 536.8 | 51.75 | 0.254 |
| 1-Butanol | 74.123 | 0.594 | 563.1 | 44.23 | 0.26 |
| 1-Hexanol | 102.177 | 0.579 | 611.4 | 35.1 | 0.263 |
| 2-Propanol | 60.096 | 0.668 | 508.3 | 47.62 | 0.248 |
| Phenol | 94.113 | 0.444 | 694.3 | 61.3 | 0.243 |
| Ethylene glycol | 62.068 | 0.487 | 719.7 | 77 | 0.246 |
| Acetic acid | 60.053 | 0.467 | 592 | 57.86 | 0.211 |
| *n*-Butyric acid | 88.106 | 0.681 | 615.7 | 40.64 | 0.232 |
| Benzoic acid | 122.123 | 0.603 | 751 | 44.7 | 0.246 |
| Acetonitrile | 41.053 | 0.338 | 545.5 | 48.3 | 0.184 |
| Methylamine | 31.057 | 0.281 | 430.1 | 74.6 | 0.321 |
| Ethylamine | 45.084 | 0.285 | 456.2 | 56.2 | 0.307 |
| Nitromethane | 61.04 | 0.348 | 588.2 | 63.1 | 0.223 |
| Carbon tetrachloride | 153.822 | 0.193 | 556.4 | 45.6 | 0.272 |
| Chloroform | 119.377 | 0.222 | 536.4 | 54.72 | 0.293 |
| Dichloromethane | 84.932 | 0.199 | 510 | 60.8 | 0.265 |
| Methyl chloride | 50.488 | 0.153 | 416.3 | 66.8 | 0.276 |
| Ethyl chloride | 64.514 | 0.19 | 460.4 | 52.7 | 0.275 |
| Chlorobenzene | 112.558 | 0.25 | 632.4 | 45.2 | 0.265 |
| Neon | 14.0099 | 0 | 44.4 | 27.6 | 0.311 |
| Argon | 39.948 | 0 | 150.9 | 48.98 | 0.291 |
| Krypton | 83.8 | 0 | 209.4 | 55.02 | 0.288 |
| Xenon | 165.03 | 0 | 289.7 | 58.4 | 0.286 |
| Helium 4  Hydrogen | 4.003  2.016 | -0.39 | 5.2  33.19 | 2.28  13.13 | 0.302  0.305 |
| Oxygen | 31.999 | 0.022 | 154.6 | 50.43 | 0.288 |
| Nitrogen | 28.014 | 0.038 | 126.2 | 34 | 0.289 |
| Chlorine | 70.905 | 0.069 | 417.2 | 77.1 | 0.265 |
| Carbon monoxide | 28.01 | 0.048 | 132.9 | 34.99 | 0.299 |
| Carbon dioxide | 44.01 | 0.224 | 304.2 | 73.83 | 0.274 |
| Carbon disulﬁde | 76.143 | 0.111 | 552 | 79 | 0.275 |
| Hydrogen sulﬁde | 34.082 | 0.094 | 373.5 | 89.63 | 0.284 |
| Sulfur dioxide | 64.065 | 0.245 | 430.8 | 78.84 | 0.269 |

-0.216

(*continued* )

VAPOR-PRESSURE EQUATION CONSTANTS 305

Table A.1 (*Continued*)

Molar Mass

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sulfur trioxide | (¼ Molecular Weight) *M* (g/mol)  80.064 | v  0.424 | *Tc*(K)  490.9 | *Pc* (bar)  82.1 | *zc*  0.255 |
| Nitric oxide (NO) | 30.006 | 0.583 | 180.2 | 64.8 | 0.251 |
| Nitrous oxide (N2O) | 44.013 | 0.141 | 309.6 | 72.45 | 0.274 |
| Hydrogen chloride | 36.461 | 0.132 | 324.7 | 83.1 | 0.249 |
| Hydrogen cyanide | 27.026 | 0.41 | 456.7 | 53.9 | 0.197 |
| Water | 18.015 | 0.345 | 647.1 | 220.55 | 0.229 |
| Ammonia | 17.031 | 0.253 | 405.7 | 112.8 | 0.0242 |
| Nitric acid | 63.013 | 0.714 | 520 | 68.9 | 0.231 |

Sulfuric acid 98.08 \*\*\*\* 924 64 0.147

*Source:* From Smith, J. M., H. C. van Ness, and M. M. Abbot, *Introduction to Chemical Engineering Thermodynamics*, ed. 5. New York: McGraw-Hill (1996). Reproduced with permission of the McGraw-Hill Companies.

# VAPOR-PRESSURE EQUATION CONSTANTS

Table A.2 gives the Antoine equation constants for

*B* are not changed. We also see it with ln *p* instead of log *p* and with *p* expressed in psia, bar, or atm. Changing from one of those forms to the other requires simple multiplication of

## *B*

log *p* ¼ *A*- *T* þ *C* ; *p* in mm Hg; *T* in

We often see this equation as

## *B*

0C ðA:1Þ

*A* and *B* by suitable constants.

The original sources often give temperature ranges over which these constants should be used. However, we can normally extrapolate beyond those ranges, with only modest loss of accuracy. Most of these constants reproduce

log *p* ¼ *A*- *T*-*C* ; *p* in mm Hg; *T* in K ðA:2Þ

The *C* in Eq. A.2 is [273.15 minus the *C* in Eq. A.1]; the *A* and

the temperature region near the NBP very well, tempera- tures far above and below the NBP not as well (see Figure 5.5).

Table A.2 Antoine Equation Constants

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Substance | Formula | A | B | C |
| Acetaldehyde | C2H4O | 7.05648 | 1070.60 | 236 |
| Acetic acid | C2H4O2 | 7.29964 | 1479.02 | 216.81 |
| Acetone | C3H6O | 7.02447 | 1161 | 224 |
| Acetylene | C2H2 | 7.09990 | 711.00 | 253.38 |
| Ammonia | NH3 | 7.36048 | 926.13 | 240.17 |
| Argon | Ar | 6.61562 | 304.2283 | 267.31 |
| Benzene | C6H6 | 6.90565 | 1211.033 | 220.79 |
| *n*-Butane | C4H10 | 6.80897 | 935.86 | 238.73 |
| *n*-Butanol | C4H10O | 7.838 | 1558.190 | 196.881 |
| Carbon dioxide, solid | CO2(s) | 9.81064 | 1347.788 | 272.99 |
| Carbon dioxide, liquid | CO2(l) | 7.5788 | 863.35 | 273.15 |
| Carbon monoxide, | CO | 6.24021 | 230.272 | 260 |
| Carbon tetrachloride | CCl4 | 6.9339 | 1242.43 | 230 |
| Chlorine | Cl2 | 6.9317 | 859.17 | 246.14 |
| Chlorobenzene | C6H5Cl | 6.9781 | 1431.06 | 217.55 |
| Chloroform | CHCl3 | 6.9547 | 1170.97 | 226.23 |
| Cyclohexane | C6H12 | 6.84132 | 1201.53 | 222.65 |
| Ethane | C2H6 | 6.80267 | 656.4028 | 255.99 |
| Ethyl acetate | C4H8O2 | 7.01457 | 1211.90 | 216  (*continued* ) |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 306 APPENDIX A: USEFUL TABLES | AND CHARTS |  | | |
| Table A.2 (*Continued*) |  |
| Substance | Formula | A | B | C |
| Ethyl alcohol | C2H6O | 8.04494 | 1554.3 | 222.65 |
| Ethylbenzene | C8H10 | 6.95719 | 1424.255 | 213.206 |
| Ethylene | C2H4 | 6.74756 | 585.00 | 255 |
| Fluorine | F2 | 6.80540 | 310.130 | 267.15 |
| Helium | He | 5.32072 | 14.6500 | 274.94 |
| Hydrogen | H2 | 5.92088 | 71.6153 | 276.34 |
| Hydrogen chloride | HCl | 7.16761 | 744.490 | 258.7 |
| Isopropyl alcohol | C3H8O | 8.11822 | 1580.92 | 219.61 |
| Isopentane | C5H12 | 6.78967 | 1020.012 | 233.097 |
| Lead | Pb | 7.827 | 9845.4 | 273.15 |
| Mercury | Hg | 7.8887 | 3148.0 | 273.15 |
| Methane | CH4 | 6.61184 | 389.9278 | 265.99 |
| Methyl alcohol | CH4O | 8.07247 | 1574.99 | 238.86 |
| Methyl ethyl ketone | C4H8O | 6.97421 | 1209.6 | 216 |
| *n*-Decane | C10H22 | 6.95367 | 1501.2724 | 194.48 |
| *n*-Heptane | C7H16 | 6.9024 | 1268.115 | 216.9 |
| *n*-Hexane | C6H14 | 6.87776 | 1171.53 | 224.366 |
| *n*-Pentane | C5H12 | 6.85221 | 1064.63 | 232 |
| Neon | Ne | 6.08443 | 78.37729 | 270.54 |
| Nitric oxide | NO | 8.74295 | 682.9382 | 268.27 |
| Nitrogen | N2 | 6.49454 | 255.6784 | 266.55 |
| Nitrogen dioxide | NO2 | 8.91717 | 1798.543 | 276.8 |
| Oxygen | O2 | 6.69147 | 319.0117 | 266.7 |
| Ozone | O3 | 6.83670 | 552.5020 | 250.99 |
| Propane | C3H8 | 6.82970 | 813.2008 | 247.99 |
| Styrene | C8H8 | 6.92409 | 1420 | 206 |
| Toluene | C7H8 | 6.95334 | 1343.943 | 219.377 |
| Water | H2O | 7.94917 | 1657.462 | 227.02 |
| *o*-Xylene | C8H10 | 6.99893 | 1474.68 | 213.69 |

*Source.* These values are taken from a variety of sources. Longer lists are in Dean, J. A. *Lange’s Handbook of Chemistry,* ed. 12. New York. McGraw–Hill, pp. 10–29 to 10–54 (1979); Reid, R. C., J. M. Prausnitz, and T. K. Sherwood. *The Properties of Liquids and Gases,* ed. 3. New York: McGraw-Hill, Appendix A (1977); and Lide, D. R., ed. *CRC Handbook of Chemistry and Physics,* ed. 71. Boca Raton, FL: CRC Press, pp. 6–70 (1990).

# HENRY’S LAW CONSTANTS

Henry’s law

common temperatures. All values are in atmospheres x 10 ; that is, the Henry’s law constant for oxygen at 00C ¼ 2.55 x 104 atm ¼ 25,500 atm.

*y xi* · *Hi*

4

¼

*i*

*P*

ð3:6Þ

To make life hard for the student and the working engi-

neer, Henry’s law is expressed in a variety of ways, with a

is quite useful for gases well above their critical tempera-

variety of dimensions. We can rewrite Eq. 3.6 as

tures, dissolved in liquids. It is less applicable for gases at or near their critical temperatures like ethane or CO2, and more reliable for gases that do not ionize in the liquid, like oxygen

*H*

*i* ¼ *P* ·

*y i*

concentration of dissolved gas; in some set of units

ðA:3Þ

in water, than for those that do ionize, like carbon dioxide in water. It is applicable for gases dissolved in any liquid, but most of the published Henry’s law constants are for gases in water. A high value of *Hi* indicates a low solubility of the gas.

( )

If the concentration is expressed in mol fraction, then Eq. A.3 is the same as Eq. 3.6. But we regularly see g/L, mol/L, g/kg, mol/kg, lb/ft3, and lbmol/ft3 as the concentration units. For dilute aqueous solutions, for which

Henry’s law is introduced in Chapter 3 and discussed in more kg

1000 g=*L*

mol

detail in Chapter 9.

Table A.3 gives the reported values of the Henry’s law constant *H* for a variety of gases *dissolved in water* at

r 1:00 L and rmolar; solvent 18:015 g=*mol* ¼ 55:5 L

ðA:AÞ

FUGACITY COEFFICIENT CHARTS 307

the concentration of dissolved gas is Chemists regularly write Henry’s law as

mol

*c* ¼ *x* · 55:5

( a different kind of Henry0s )

so that

*i i* L

*xi* ¼

law constant

· *Pyi* ðA:CÞ

*H*Eq:A:3 ¼ 55:5

mol

L · *H*Eq:3:6 ðA:BÞ

This Henry’s law constant is the reciprocal of the one used in

this book.

Table A.3 Henry’s Law Constants for Common Gases in Water

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | | | | *T* (0C) |  | | |
|  | 0 | 10 | 20 |  | 30 | 40 | 50 |
| Acetylene | 0.072 | 0.096 | 0.121 |  | 0.146 |  |  |
| Carbon dioxide | 0.073 | 0.105 | 0.148 |  | 0.194 | 0.251 | 0.321 |
| Ethane | 1.26 | 1.89 | 2.63 |  | 3.42 | 4.23 | 5.00 |
| Helium | 12.9 | 12.6 | 12.5 |  | 12.4 | 12.1 | 11.5 |
| Hydrogen | 5.79 | 6.36 | 6.83 |  | 7.29 | 7.51 | 7.65 |
| Hydrogen sulﬁde | 0.0268 | 0.0367 | 0.0483 |  | 0.0609 | 0.0745 | 0.0884 |
| Methane | 2.24 | 2.97 | 3.76 |  | 4.49 | 5.20 | 5.77 |
| Nitrogen | 5.29 | 6.687 | 8.04 |  | 9.24 | 10.4 | 11.3 |
| Oxygen | 2.55 | 3.27 | 4.01 |  | 4.75 | 5.35 | 5.88 |
| Ozone | 0.194 | 0.248 | 0.376 |  | 0.598 | 1.20 | 2.74 |

*Source:* Henry’s law values (not all in the same units) are found in various editions of *Perry’s Chemical Engineers’ Handbook*, McGraw-Hill and *The Handbook of Chemistry and Physics*, CRC Press.

* 1. COMPRESSIBILITY FACTOR CHART (*z* CHART)

The basic idea of the *theorem of corresponding states* is that this plot (Figure A.4) must be the same for all gases. That is *only approximately true.* Much more accurate ways of estimating ﬂuid densities are available in our computers. But the classic compressibility factor chart (used with the values in Table A.1) allows us to make a very quick estimate of the departure from ideal gas behavior, and it gives some insight into the form of that departure.

Here

# FUGACITY COEFFICIENT CHARTS

According to the *theorem of corresponding states* this plot (Figure A.5, both forms) must be the same for all gases. That is *only approximately true.* Much more accurate ways of estimating pure-component fugacity coefﬁcients are available in our computers. But the classic fugacity coef- ﬁcient charts (used with the values in Table A.1) allow us to make a very quick estimate of the departure from ideal gas behavior, and give some insight into the form of this function.

*z* ¼ ( compressibility ) ¼ *Pv*

factor *RT*

For a ideal gas, *z* ¼ 1.

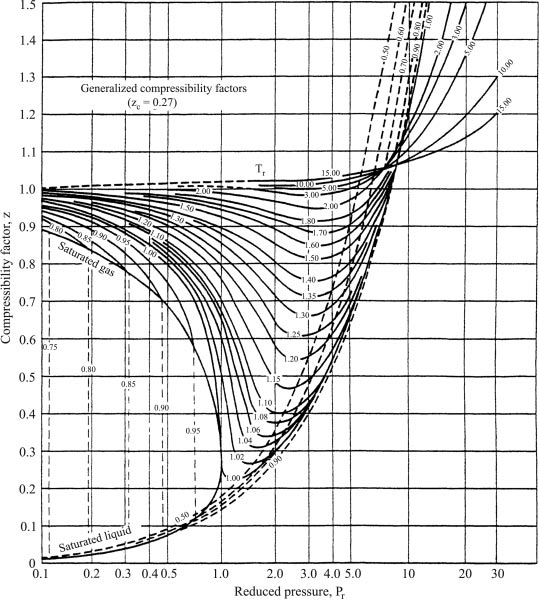


FIGURE A.4 Compressibility factor chart. (From Hougen, O. A., K. M. Watson, and R. A. Ragatz, *Chemical Process Principles*, Part II: *Thermodynamics*, ed. 2. ©1959. New York: Wiley. Reprinted by permission of the estate of O. A. Hougen.)

# AZEOTROPES

Tables A.6.1 and A.6.2 are excerpts from the longer tables in *Perry’s Chemical Engineers’ Handbook*. More exten-

sive tables can be found in *CRC Handbook of Chemistry and Physics*, and in Horsley, *Advances in Chemistry Series*. ed. 6, Washington, DC: American Chemical Society (1952).

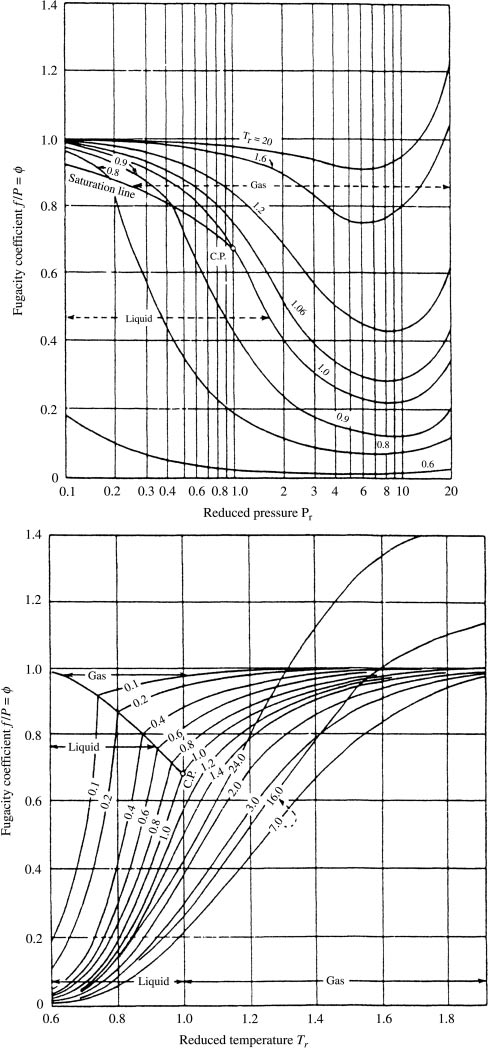


FIGURE A.5 Fugacity coefﬁcient chart. (From Hougen, O. A., K. M. Watson, and R. A. Ragatz, *Chemical Process Principles*, Part II: *Thermodynamics*, ed. 2. © 1959. New York: Wiley. Reprinted by permission of the estate of O. A. Hougen.)

Table A.6.1 Minimum Boiling Binary Azeotropes at 760 torr

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | System |  | | |
| A |  | B | Mol% A | Temperature (0C) |
| Water |  | Ethanol | 10.57 | 78.15 |
|  |  | Allyl alcohol | 54.5 | 88.2 |
|  |  | Propionic acid | 94.7 | 99.98 |
|  |  | Propyl alcohol | 56.83 | 87.72 |
|  |  | Isopropyl alcohol | 31.46 | 80.37 |
|  |  | Methyl ethyl ketone | 33 | 73.45 |
|  |  | Isobutyric acid | 94.5 | 99.3 |
|  |  | Ethyl acetate (2 phase) | 24 | 70.4 |
|  |  | Ethyl ether (2 phase) | 5 | 34.15 |
|  |  | *n*- Butyl alcohol (2 phase) | 75 | 92.25 |
|  |  | Isobutyl alcohol | 67.14 | 89.92 |
|  |  | *sec*-Butyl alcohol | 66 | 88.5 |
|  |  | *tert*-Butyl alcohol | 35.41 | 79.91 |
|  |  | Isoamyl alcohol (2 phase) | 82.79 | 95.15 |
|  |  | Amyl alcohol (tert) (2 phase) | 65 | 87 |
|  |  | Benzene (2 phase) | 29.6 | 69.25 |
|  |  | Toluene (2 phase) | 55.6 | 84.1 |
| Carbon tetrachloride |  | Methanol | 44.5 | 55.7 |
|  |  | Ethanol | 61.3 | 64.95 |
|  |  | Allyl alcohol | 73 | 72.32 |
|  |  | *n*-Propyl alcohol | 75 | 72.8 |
|  |  | Ethyl acetate | 43 | 74.75 |
| Carbon disulﬁde |  | Methanol | 72 | 37.65 |
|  |  | Ethanol | 86 | 42.4 |
|  |  | Acetone | 61 | 39.25 |
|  |  | Methyl acetate | 69.5 | 40.15 |
| Chloroform |  | Methanol | 65 | 53.5 |
|  |  | Ethanol | 84 | 59.3 |
|  |  | Isopropyl alcohol | 92 | 60.8 |
| *n*-Butyl alcohol |  | Cyclohexane | 11 | 79.8 |
|  |  | Toluene | 37 | 105.5 |
| Isobutyl alcohol |  | Isoamyl bromide | 60 | 103.8 |
|  |  | Benzene | 10 | 79.84 |
|  |  | Toluene | 50 | 101.15 |
| *n*-Amyl alcohol |  | *i*-Amyl acetate | 96.4 | 131.3 |
|  |  | *i*-Butyl propionate | 85 | 130.5 |
| Isoamyl alcohol |  | Chlorobenzene | 42 | 124.3 |
|  |  | *o*-Xylene | 64 | 128 |
|  |  | *m*-Xylene | 58 | 127 |
|  |  | *p*-Xylene | 56 | 126.8 |
| Nitrobenzene |  | Benzyl alcohol | 39 | 204.3 |
| Phenol |  | *p*-Bromotoluene | 58 | 176.2 |
| Acetic acid |  | Chlorobenzene | 72.5 | 114.65 |
|  |  | Benzene | 2.5 | 80.05 |
|  |  | Toluene | 62.7 | 105.4 |
|  |  | *m*-Xylene | 40 | 115.38 |
| Ethyl alcohol |  | Methyl ethyl ketone | 45 | 74.8 |
|  |  | Ethyl acetate | 46 | 71.8 |
|  |  | Methyl propionate | 67.5 | 73.2 |
|  |  | *n*-Propyl formate | 72 | 73.5 |
|  |  | Benzene | 44.8 | 68.24 |
|  |  | Cyclohexane | 44.5 | 64.9 |
|  |  | *n*-Hexane | 33.2 | 58.68 |
|  |  | Toluene | 81 | 76.65 |
|  |  | *n-*Heptane | 67 | 72 |
|  |  |  |  | (*continued* ) |

Table A.6.1 (*Continued*)

System

A B Mol% A Temperature (0C)

|  |  |  |  |
| --- | --- | --- | --- |
| Allyl alcohol | Benzene | 22.2 | 76.75 |
|  | Cyclohexane | 26.6 | 74 |
|  | *n-* Hexane | 6.5 | 65.5 |
|  | Toluene | 61.5 | 92.4 |
| Acetone | Methyl acetate | 61 | 56.1 |
|  | Isobutyl chloride | 81 | 55.8 |
|  | Diethylamine | 43.5 | 51.5 |
| *n*-Propyl alcohol | Ethyl propionate | 64 | 93.4 |
|  | Benzene | 20.9 | 77.12 |
|  | *n-*Hexane | 6 | 65.65 |
|  | Toluene | 60 | 92.6 |
| Isopropyl alcohol | Ethyl acetate | 30.5 | 74.8 |
|  | Benzene | 39.3 | 71.92 |
|  | *n-*Hexane | 29 | 61 |
|  | Toluene | 77 | 80.6 |
| Tetrachloroethylene | Ethanol | 6 | 77.95 |
|  | Allyl alcohol | 27 | 94 |
|  | Propionic acid | 81 | 118.95 |
|  | *n-*Propyl alcohol | 24 | 94 |
|  | Isopropyl alcohol | 8 | 81.7 |
|  | *n-*Butyl alcohol | 47 | 110 |
|  | Isobutyl alcohol | 40 | 103.05 |

*Source:* Taken from Perry R. H., and D. W. Green, eds. *Perry’s Chemical Engineer’s Handbook*, ed. 6, pp. 13–59 and 13–50, McGraw-Hill (2003).

Table A.6.2 Maximum Boiling Binary Azeotropes at 760 torr

System

|  |  |  |  |
| --- | --- | --- | --- |
| A | B | Mol% A | Temperature (0C) |
| Water | Hydroﬂuoric acid | 65.4 | 120 |
|  | Hydrochloric acid | 88.9 | 110 |
|  | Perchloric acid | 32 | 203 |
|  | Hydrobromic acid | 83.1 | 126 |
|  | Hydriodic acid | 84.3 | 127 |
|  | Nitric acid | 62.2 | 120.5 |
|  | Formic acid | 43.3 | 107.1 |
| Chloroform | Acetone | 65.5 | 64.5 |
| Formic acid | Diethyl ketone | 48 | 105.4 |
|  | Methyl propyl ketone | 47 | 105.3 |
| Phenol | Cyclohexanol | 90 | 182.45 |
|  | Benzaldehyde | 54 | 185.6 |
|  | Benzyl alcohol | 8 | 206 |
| *o-* Cresol | Acetophenone | 24 | 203.7 |
|  | Phenyl acetate | 42.5 | 198.6 |
|  | Methyl hexyl ketone | 97 | 191.5 |
|  | Isoamyl butyrate | 80 | 192 |
| *m*-Cresol | Acetophenone | 54 | 209 |
|  | Isoamyl lactate | 60 | 207.6 |
| *p–*Cresol | Benzyl alcohol | 38 | 207 |
|  | Acetophenone | 52 | 208.45 |

*Source:* Taken from Perry R. H., and D. W. Green, eds. *Perry’s Chemical Engineer’s Handbook*, ed. 6, pp. 13–59 and 13–50, McGraw-Hill (2003).

# VAN LAAR EQUATION CONSTANTS

Table A.7 is an excerpt from a much longer table taken from Holmes and Van Winkle, which gives the original literature citations and the corresponding constants for several other

*B*2*Ax*2

log g1 ¼ ð*Ax* þ *Bx* Þ

2

2

1 2

2 2

log g2 1

*A Bx*

2

¼

ð*Ax*1 þ *Bx*2Þ

ð8:LÞ

equations. The traditional form is

*Ax*2

2

log g1 ¼ *A* 2 log g2 ¼

( ) (

*x*1 þ *x*2

*B*

*Bx*2

*B* 2

1

)

*x*1 þ *A x*2

ð8:12Þ

These are in the log form. We also often see this equation in

the ln form (ln g1 etc.) for which the constants *A* and *B* are

¼

2.303 times as large as those shown here. We must always check to see which form the reported constants correspond to. Most of the values in this table are for data at a constant pressure of 760 torr. Some are constant temperatures, as shown. As discussed in Chapter 9, there should not be much difference between the constants obtained either way, which is observed for most of the pairs in this table for which both

forms are shown.

Some pairs, such as acetone–water, are shown twice, once with acetone as component 1 and once with water as com-

For programming our computers the following form is simpler

ponent 1. The reader may check to see that this simply interchanges the values of *A* and *B*.

Table A.7 Van Laar Equation Constants

0.6345 0.6358

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Component 1 | Component 2 | *A* | *B* | Pressure (torr) | Temperature (0C) |
| Acetone | Benzene | 0.2039 | 0.1563 | 760 |  |
|  | Carbon tetrachloride | 0.3889 | 0.3301 | 760 |  |
|  | Chloroform  2,3-Dimethylbutane Ethanol | -0.3045  0.2574 | -0.2709  0.2879 | 760  760  760 |  |
|  | Methanol  *n*-Pentane | 0.2635  0.2763  0.7403 | 0.2801  0.2878  0.6364 | 760  760 | 55 |
|  | 2-Propanol  Water | 0.2186  0.3158  0.9972 | 0.269  0.2495  0.6105 | 760  760 | 55 |
| Acetonitrile | Water | 1.068 | 0.8207 | 760 |  |
| Benzene | Acetone | 0.1563 | 0.2039 | 760 |  |
|  | 1-Butanol | 0.3594 | 0.5865 | 760 |  |
|  | Carbon tetrachloride | 0.036 | 0.0509 | 760 |  |
|  | Chloroform Cyclohexane  Cyclopentane | -0.0858  0.1655 | -0.0556  0.1302 | 760  760  760 |  |
|  | Ethanol  *n*-Heptane  *n*-Hexane | 0.5804  0.0985  0.1072  0.1457 | 0.7969  0.2135  0.2361  0.2063 | 760  760  760 | 75 |
|  | Methanol | 0.7518 | 0.8975 | 760 |  |
|  | Methyl acetate | 0.1292 | 0.0919 | 760 |  |
|  | Methylcyclohexane | 0.091 | 0.1901 | 760 |  |
|  | Methylcyclopentane | 0.136 | 0.1605 | 760 |  |
|  | 1-Propanol  2-Propanol | 0.3772  0.4508  0.4638 | 0.7703  0.7564  0.6723 | 760  760 | 75 |
|  |  | 0.5455 | 0.7716 | 500 |  |
| 1-Butanol | Benzene | 0.5865 | 0.3594 | 760 |  |
|  | Toluene | 0.543 | 0.3841 | 760 | (*continued* ) |

0.1466 0.1646

Table A.7 (*Continued*)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Carbon tetrachloride | Acetone | 0.3301 | 0.3889 | 760 |
|  | Benzene | 0.0509 | 0.036 | 760 |
|  | 2-Propanol | 0.4918 | 0.7868 | 760 |
| Chloroform | Acetone  Benzene | -0.2709 | -0.3045 | 760  760 |
|  | 2,3-Dimethylbutane | 0.1736 | 0.279 | 760 |
|  | Ethyl acetate | -0.2868 | -0.4478 | 760 |

Component 1 Component 2 *A B* Pressure (torr) Temperature (0C)

-0.0556 -0.0858

Methanol 0.4104 0.8263 760

Methyl acetate -0.2249 -0.3343 760

Methyl ethyl ketone -0.299 -0.3486 760

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Water | Acetone | 0.6105 | 0.9972 | 760 |  |
|  | Acetonitrile | 0.8207 | 1.0680 | 760 |
|  | Ethanol | 0.4104 | 0.7292 | 760 |
|  | Methanol | 0.2439 | 0.3861 | 760 |
|  | 1-Propanol | 0.5037 | 1.1433 | 760 |
|  |  | 0.5305 | 1.2315 |  | 40 |
|  |  | 0.5224 | 1.1879 |  | 60 |
|  | 2-Propanol | 0.4750 | 1.0728 | 760 |  |
|  | *n*-butanol | 0.5531 | 1.7269 | 760 |  |

*Source:* Taken from Holmes, M. J., and M. van Winkle, Prediction of ternary vapor-liquid from binary data. *Ind. Eng. Chem.* 62:21–31 (1970).

# ENTHALPIES AND GIBBS ENERGIES OF FORMATION FROM THE ELEMENTS IN THE STANDARD STATES, AT *T* ¼ 298.15 K ¼ 250C, AND P ¼ 1.00 BAR

The standard states in Table A.8 are (g), pure ideal gas at 1 bar; (l) and (s), the normal state of that substance at 1 bar

and 250C; (aq), an ideal 1-molal solution of that substance in water at 1 bar and 250C. For several substances, such as water, values are shown for two standard states, (1) and (g).

The relation between these is shown in Example 12.7.

Table A.8 Enthalpies and Gibbs Energies of Formation from the Elements

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Chemical Species | Formula | State | *h*0 of Formation from the Elements (kJ/mol) | *g*0 of Formation from the Elements (kJ/mol) |
| PARAFFINIC HYDROCARBONS  Methane | CH4 | (g) | -74.5 | -50.5 |

Ethane C2H6 (g) -83.8 -31.9

Propane C3Hg (g) -104.7 -24.3

*n*-Butane C4H10 (g) -125.8 -17.2

Isobutane C4H10 (g) -134.5 -20.9

*n*-Pentane C5H12 (g) -146.8 -8.7

*n*-Pentane C5H12 (1) -173.1 9.2

*n*-Hexane C6H14 (l) -166.9 0.2

*n*-Heptane C7H16 (g) -187.8 8.3

*n*-Octane C8H18 (g) -208.8 16.3

*n*-Octane C8H18 (I) -255.1

UNSATURATED HYDROCARBONS

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Acetylene | C2H2 | (g) | 227.5 | 210.0 |
| Ethylene | C2H4 | (g) | 52.5 | 68.5 |
| Propylene | C3H6 | (g) | 19.7 | 62.2 |
| 1-Butene | C4H8 | (g) | 1.2 | 70.3 |
| 1-Pentene | C5H10 | (g) | -21.3 | 78.4 |
| 1-Hexene C6H12  1-Heptene C7H14 | | (g) -42.0 86.8  (g) -62.3 95.8 | | |
| 1,3-Butadiene C4H6 | | (g) 109.2 149.8 | | |

(*continued* )

Chemical Species Formula State

*h*0 of Formation from the Elements (kJ/mol)

*g*0 of Formation from the Elements (kJ/mol)

AROMATIC HYDROCARBONS

Benzene C6H6 (g) 82.9 129.7

Benzene C6H6 (l) 49.1 124.5

Ethylbenzene C8H10 (g) 29.9 130.9

Naphthalene C10H8 (g) 1501.0 223.6

Styrene C8H8 (g) 147.4 213.9

Toluene C7H8 (g) 50.2 122.1

Toluene C7H8 (1) 12.2 113.6

CYCLIC HYDROCARBONS

Cyclohexane C6H12 (g) -123.1 31.9

Cyclohexane C6H12 (l) -156.2 26.9

Cyclopropane C3H6 (g) 53.3 104.5

*methyl*-Cyclohexane C7H14 (g) -154.8 27.5

*methyl*-Cyclohexane C7H14 (1) -190.2 20.6

Cyclohexene C6H10 (g) -5.4 106.9

OXYGENATED HYDROCARBONS

Acetaldehyde C2H4O (g) -166.2 -128.9

Acetic acid CH3COOH (l) -484.5 -389.9

Acetic acid CH3COOH (aq) -486.1 -396.5

1,2-Ethanediol (ethylene glycol) C2H6O2 (1) -454.8 -323.1

Ethanol C2H6O (g) -235.1 -168.5

Ethanol C2H6O (l) -277.7 -174.8

Ethyl acetate CH3COOC2H5 (l) -463.3 -318.4

Ethylene oxide C2H4O (g) -52.6 -13.0

Formaldehyde CH2O (g) -108.6 102.5

Formic acid HCOOH (l) -424.7 -361.4

Methanol CH4O (g) -200.7 -162.0

Methanol CH4O (1) 238.7 -166.3

Phenol C6H5OH (g) -165.0 -50.9

INORGANIC COMPOUNDS

Aluminum oxide Al2O3 (s, a) -1675.7 -1582.3 Aluminum chloride AlCl3 (s) -704.2 -628.8

Ammonia NH3 (g) -46.1 -16.5

Ammonia NH3 (aq) -80.3 -26.6

Ammonium nitrate NH4NO3 (s) -365.6 -183.9

Ammonium chloride NH4Cl (s) -314.4 -202.9

Barium oxide BaO (s) -553.5 -525.1

Barium chloride BaCl2 (s) -856.6 -810.4

Bromine Br2 (l) 0 0

Bromine Br2 (g) 30.9 3.1

Calcium carbide CaC2 (s) -59.8 -64.9

Calcium carbonate CaCO3 (s) -1206.9 -1128.8

Calcium chloride CaCl2 (s) -795.8 -748.1

Calcium chloride CaCl2 (aq) -8101.9 Calcium chloride hexahydrate CaCl2 · 6H2O (s) -2607.9

Calcium hydroxide Ca(OH)2 (s) -986.1 -898.5

Calcium hydroxide Ca(OH)2 (aq) 1002.82 868.1

- -

Calcium oxide CaO (s) 635.1 604.0

- -

Carbon (graphite) C (s) 0 0

Carbon (diamond) C (s) 1.9 2.9

Carbon dioxide CO2 (g) - 393.5 -394.4

Carbon dioxide CO2 (aq) -413.8 -386.0

Carbon disulﬁde CS2 (l) 89.7 65.3

(*continued* )

Carbon tetrachloride CCl4 (l) -135.4 -65.2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Table A.8 (*Continued*) |  | | | |
| Chemical Species | Formula | State | *h*0 of Formation from the Elements (kJ/mol) | *g*0 of Formation from the Elements (kJ/mol) |
| Carbon monoxide | CO | (g) | -110.5 | -137.2 |

Carbonic acid H2CO3 (aq) 699.7 623.1

-

Hydrochloric acid HCl (g) 92.3 95.3

- -

Hydrochloric acid HC1 (aq) 167.2 131.2

- -

Hydrogen bromide HBr (g) 36.4 53.5

- -

Hydrogen cyanide HCN (g) 135.1 124.7

Hydrogen cyanide HCN (l) 108.9 125.0

Hydrogen ﬂuoride HF (g) 271.1 273.2

- -

Hydrogen iodide HI (g) 26.5 1.7

Hydrogen peroxide H2O2 (l) -187.8 -120.4

Hydrogen sulﬁde H2S (g) -20.6 -33.6

Hydrogen sulﬁde H2S (aq) -39.7 -27.8

Iodine I2 (g) 62.3 19.8

Iodine I2 (s) 0 0

Iron (II) oxide FeO (s) -272.0

Iron (III) oxide (hematite) Fe2O3 (s) -824.2 -742.2 Iron (II) sulﬁde FeS (s, /) -100.0 -100.4 Iron sulﬁde (pyrite) FeS2 (s) 178.2 166.9

Lead oxide PbO (s, yellow) -217.3 -187.9

Lead oxide PbO (s, red) -219.0 -188.9

Lead dioxide PbO2 (s) -277.4 -217.3

Lead sulfate PbSO4 (s) -919.9 -813.2

Lithium chloride LiCl (s) -408.6 -216.7

Lithium chloride LiCl · H2O (s) -712.6 -631.8

Lithium chloride LiCl · 2H2O (s) -1012.7

Lithium chloride LiCl · 3H2O (s) -1311.3

Lithium ﬂuoride LiF (s) -615.96 587.7

Magnesium oxide MgO (s) -601.7 -569.4

Magnesium carbonate MgCO3 (s) -1095.8 -1012.1

Magnesium chloride MgCl2 (s) -641.3 -591.8 Mercury (I) chloride Hg2Cl2 (s) -265.2 -210.8 Mercury (II) chloride HgCl2 (s) -224.3 -178.6 Nitric Acid HNO3 (l) -174.1 -80.7

Nitric Acid HNO3 (aq) 207.4 111.3

- -

Nitric oxide NO (g) 90.3 86.6

Nitrogen dioxide NO2 (g) 33.2 51.3

Nitrous oxide N2O (g) 82.1 104.2

Nitrogen tetroxide N2O4 (g) 9.2 97.9

Potassium chloride KCl (s) -436.8 -409.1 Silicon dioxide SiO2 (s, a) -910.9 -856.6

Silver bromide AgBr (s) -100.4 -96.9

Silver chloride AgCl (s) -127.1 -109.8

Silver nitrate AgNO3 (s) -124.4 -33.4

Sodium bicarbonate NaHCO3 (s) -945.6 -847.9

Sodium carbonate Na2CO3 (s) -1130.7 -1044.4 Sodium carbonate decahydrate Na2CO3 · 10H2O (s) -4081.3 -3428,2 Sodium chloride NaCl (s) -411.2 -384.1

Sodium chloride NaCl (aq) -393.1 Sodium hydroxide NaOH (s) -425.6 -379.5 Sodium hydroxide NaOH (aq) -419.2 Sodium sulfate Na2SO4 (s) -1382.8 -1265.2 Sodium sulfate decahydrate Na2SO4 10H2O (s) 4322.5 3642.3

· - -

(*continued* )

Chemical Species Formula State

*h*0 of Formation from the Elements (kJ/mol)

*g*0 of Formation from the Elements (kJ/mol)

Sulfur S2 (g) 129.8 81.0

Sulfur S2 (l) 1.1 0.3

Sulfur S2 (s) 0 0

Sulfur dioxide SO2 (g) -296.8 -300.2

Sulfur dioxide SO2 (aq) -323.0 -300.7

Sulfur trioxide SO3 (g) -395.73 -371.1

Sulfur trioxide SO3 (1) -441.0 -368.4

Sulfuric acid H2SO4 (l) -814.0 -690.0

Sulfuric acid H2SO4 (aq) -909.3 -744.5

Sulfurous acid H2SO3 (aq) -608.8 537.9

Water H2O (g) 241.8 -228.6

Water H2O (l) -285.8 -237.1

Zinc oxide ZnO (s) -348.3 -318.3

IONS

Hydrogen Hþ (aq) 0 0

Aluminum Al3þ (aq) -531.37 -485.34

Ammonium NH4þ

(aq) -132.51 - 79.37

Calcium Ca2þ (aq) 542.83 553.54

- -

Cupric Cu2þ (aq) 64.77 65.52

Cuprous Cuþ (aq) 71.67 50.00

Ferric Fe3þ (aq) 48.53 4.60

- -

Ferrous Fe2þ (aq) 89.12 78.87

- -

Lead Pb2þ (aq) 1.67 24.39

- -

Lithium Liþ (aq) 278.49 293.3

- -

Magnesium Mg2þ (aq) 466.85 454.80

- -

Potassium Kþ (aq) 252.38 283.26

- -

Silver Agþ (aq) 105.57 77.12

Sodium Naþ (aq) -240.12 -261.66

Zinc Zn2þ (aq) -153.89 -147.03

Bicarbonate HCO-3 (aq) -691.99 -586.85

Bisulfate HSO-4 (aq) -887.34 -756.01

Bisulﬁde HS- (aq) -17.7 12.6

Bisulﬁte HSO-3 (aq) 626.2 -527.8

Bromide Br- (aq) -121.54 -103.97

Carbonate CO2-

3

(aq) -677.14 -527.89

Chloride Cl- (aq) -167.16 -131.26

Fluoride F- (aq) -332.63 -278.82

Hydroxyl OH- (aq) -229.99 -157.29

Iodide I- (aq) -55.19 -51.59

Nitrate NO-3 (aq) -207.36 -111.34

Perchlorate ClO-4 (aq) -10.8

Sulfate SO2-

4

(aq) -909.3 -744.62

Sulﬁde S2- (aq) þ 30.1 þ 79.5

Suﬁte SO2-

3

(aq) -635.5 -486.6

*Sources:* Taken from Perry R. H., and D.W. Green, eds. *Perry’s Chemical Engineer’s Handbook*, ed. 6, pp. 13–59 and 13–50, McGraw-Hill (2003); D. R. Lide, *CRC Handbook of Chemistry and Physics*. Boca Raton, FL: CRC Press.

HEAT CAPACITIES OF GASES IN THE IDEAL GAS STATE 317

# HEAT CAPACITIES OF GASES IN THE IDEAL GAS STATE

For ideal gases, *CP* is independent of pressure; for real gases at modest pressures it is almost independent of

pressure. Table A.9 shows the constants in the equation

*CP*/*R* ¼ *a* þ *bT* þ *cT*2 þ *dT* -2; *T* in K, up to *T*max.

Table A.9 Heat Capacity Equation Constants

Chemical Species Formula *T*max *a* 103*b* 106*c* 10-5*d*

PARAFFINS

Methane CH4 1500 1.702 9.081 -2.164

Ethane C2H6 1500 1.131 19.225 -5.561

Propane C3H8 1500 1.213 28.785 -8.824

*n*-Butane C4H10 1500 1.935 36.915 -11.402

Isobutane C4H10 1500 1.677 37.853 -11.945

*n*-Pentane C5H12 1500 2.464 45.351 -14.111

*n*-Hexane C6H14 1500 3.025 53.722 -16.791

*n*-Heptane C7H16 1500 3.570 62.127 -19.486

*n*-Octane C8H18 1500 8.163 70.567 22.208

-

1-ALKENES

Ethylene C2H4 1500 1.424 14.394 -4.392

Propylene C3H6 1500 1.637 22.706 6.915

1-Butene C4H8 1500 1.967 31.630 -9.873

1-Pentene C5H10 1500 2.691 39.753 -12.447

1-Hexene C6H12 1500 3.220 48.189 -15.157

1-Heptene C7H14 1500 3.768 56.588 -17.847

MISCELLANEOUS ORGANICS

Acetaldehyde C2H4O 1000 1.693 17.978 -6.158

Acetylene C2H2 1500 6.132 1.952 -1.299

Benzene C6H6 1500 -0.206 39.064 -13.301

1,3-Butadiene C4H6 1500 2.734 26.786 -8.882

Cyclohexane C6H12 1500 -3.876 63.249 -20.928

Ethanol C2H6O 1500 3.518 20.001 -6.002

Ethylbenzene C8H10 1500 1.124 55.380 -18.476

Formaldehyde CH2O 1500 2.264 7.022 -1.877

Methanol CH4O 1500 2.211 12.216 -3.450

Toluene C7H8 1500 0.290 47.052 -15.716

Styrene C8H8 1500 2.050 50.192 -16.662

MISCELLANEOUS INORGANICS

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Air |  | 2000 | 3.355 | 0.575 -0.016 |
| Ammonia | NH3 | 1800 | 3.578 | 3.020 -0.186 |
| Bromine | Br2 | 3000 | 4.493 | 0.056 -0.154 |
| Carbon monoxide | CO | 2500 | 3.376 | 0.557 -0.031 |
| Carbon dioxide | CO2 | 2000 | 5.457 | 1.045 -1.157 |
| Carbon disulﬁde | CS2 | 1800 | 6.311 | 0.805 -0.906 |
| Chlorine | Cl2 | 3000 | 4.442 | 0.089 0.344 |
| Hydrogen | H2 | 3000 | 3.249 | 0.422 0.083 |
| Hydrogen sulﬁde | H2S | 2300 | 3.931 | 1.490 -0.232 |
| Hydrogen chloride | HCl | 2000 | 3.156 | 0.623 0.151 |
| Hydrogen cyanide | HCN | 2500 | 4.736 | 1.359 0.725 |
| Nitrogen | N2 | 2000 | 3.280 | 0.593 0.040 |
| Nitrous oxide | N2O | 2000 | 5.328 | 1.214 -0.928 |
| Nitric oxide | NO | 2000 | 3.387 | 0.629 0.014 |
| Nitrogen dioxide | NO2 | 2000 | 4.982 | 1.195 -0.792 |
| Oxygen | O2 | 2000 | 3.639 | 0.506 -0.227 |
| Sulfur dioxide | SO2 | 2000 | 5.699 | 0.801 -1.015 |
| Water | H2O | 2000 | 3.470 | 1.450 0.121 |

*Sources:* Taken from Smith, J. M., H. C. van Ness, and M. M. Abbott, *Introduction to Chemical Engineering Thermodynamics*, ed. 5. New York: McGraw-Hill (1996) based on H.M. Spencer, *Ind. Eng. Chem.* 40: 2152–2154 (1948), K.K. Kelly, *U.S. Bur. Mines Bull. 584* (1960) and L.B. Pankratz, *U.S. Bur. Mines Bull. 672* (1982).