Diffusivity from the Chapman-Enskog can (1)

Source: "The Properties of Gases and Cipulds"

[Reid + She wood]

Appendix C

## Lennard-Jones Potentials as Determined from Viscosity Data<sup>†</sup>

Subs	tance <sup>-</sup>	cm³/g-mol	$\sigma$ , Å	$\epsilon/k$ , K
Ar	Argon	46.08	3.542	93.3
He	Helium	20.95	2.5518	10.22
Kr	Krypton	61.62	3.655	178.9
Ne	Neon	28.30	2.820	32.8
Xe	Xenon	83.66	4.047	231.0
Air	Air	64.50	3.711	78.6
$AsH_3$	Arsine	89.88	4.145	259.8
$BCl_3$	Boron chloride	170.1	5.127	337.7
BF <sub>3</sub>	Boron fluoride	93.35	4.198	186.3
$B(OCH_3)_3$	Methyl borate	210.3	5.503	396.7
$\mathrm{Br}_2$	Bromine	100.1	4.296	507.9
CCL	Carbon tetrachloride	265.5	5.947	322.7
$CF_4$	Carbon tetrafluoride	127.9	4.662	134.0
CHCl₃	Chloroform	197.5	5.389	340.2
$CH_2Cl_2$	Methylene chloride	148.3	4.898	356.3
CH₃Br	Methyl bromide	88.14	4.118	449.2
CH <sub>3</sub> Cl	Methyl chloride	92.31	4.182	350
CH₃OH	Methanol	60.17	3.626	481.8
CH <sub>4</sub>	Methane	66.98	3.758	148.6
CO	Carbon monoxide	63.41	3.690	91.7
COS	Carbonyl sulfide	88.91	4.130	336.0
$CO_2$	Carbon dioxide	77.25	3.941	195.2
$CS_2$	Carbon disulfide	113.7	4.483	467
$C_2H_2$	Acetylene	82.79	4.033	231.8
$C_2H_4$	Ethylene	91.06	4.163	224.7
$C_2H_6$	Ethane	110.7	4.443	215.7
$C_2H_5Cl$	Ethyl chloride	148.3	4.898	300
C <sub>2</sub> H <sub>5</sub> OH	Ethanol	117.3	4.530	362.6
$C_2N_2$	Cyanogen	104.7	4.361	348.6
CH₃OCH₃	Methyl ether	100.9	4.307	395.0

CH₃CCH Methylacetylene 136.2 4.761 251.6 C₃H₀ Cyclopropane 140.2 4.807 248.8 C₃H₀ Propane 169.2 5.118 237.1 CH₃COCH₃ Propane 169.2 5.118 237.1 CH₃COCH₃ Acetone 122.8 4.600 560.3 CH₃COOCH₃ Acetone 132.8 4.600 560.3 CH₃COOCH₃ Methyl acetate 151.8 4.936 469.9 n-C₄H₁₀ n-Butane 130.0 4.687 531.4 c₃-C₄H₁₀ lsobutane 185.6 5.278 330. C₂-H₃OC₂-H₃ Ethyl ether 231.0 5.678 313.3 CH₃-COOC₂-H₃ Ethyl acetate 178.0 5.205 521.3 n-C₃-H₁₂ n-Pentane 244.2 5.784 341. C(CH₃-O)₃ 2,2-Dimethylpropane 340.9 6.464 193.4 C₃-C₄-H₁₂ Cyclohexane 193.2 5.349 412.4 C₃-C₄-H₁₂ Cyclohexane 298.2 6.182 297. C₃-C₄-H₁₂ Cyclohexane 298.2 6.182 297. Cl₂ Chlorine 94.65 4.217 316.4 F₅ Fluorine 47.75 3.357 112.4 HBr Hydrogen bromide 47.58 3.353 449 HCN Hydrogen cyanide 60.37 3.630 569. HCl Hydrogen fluoride 46.98 3.339 344.4 HF Hydrogen fluoride 46.98 3.339 344.4 HF Hydrogen fluoride 94.24 4.211 288. Hg Hydrogen peroxide 93.24 4.211 288. Hg Mercury 33.03 2.969 750 HgBr₂ Mercuric rohnide 165.5 5.080 686. HgCl₂ Mercuric rohnide 118.9 4.550 750 HgBr₂ Mercuric chloride 118.9 4.550 750 HgBr₂ Mercuric chloride 118.9 4.550 750 NO Nitric oxide 53.74 3.492 116. NOCI Nitrosy chloride 87.75 4.112 395. NO Nitric oxide 70.80 3.828 232. O₂ Oxygen 52.60 3.467 106. SIH₄ Silicon tetrafluoride 170.2 5.128 232. SiH₄ Silicon tetrafluoride 146.77 4.880 171. SiH₄ Silicon hydride 85.97 4.084 207.	Substance		$b_{ m o}, \ddagger  m cm^3/g-mol$	σ, Å	$\epsilon/k$ , K
C₃H₀         Cyclopropane         140.2         4.807         248.5           C₃H₃         Propane         169.2         5.118         237.           n-C₃H₂OH         n-Propyl alcohol         118.8         4.549         576.           CH₃COOCH₃         Acetone         122.8         4.600         560.5           CH₃COOCH₃         Methyl acetate         151.8         4.936         469.3           n-C₄H₁₀         n-Butane         130.0         4.687         531.4           sio-C₄H₁₀         Isobutane         185.6         5.278         330.           C₃H₃OCH₃         Ethyl ether         231.0         5.678         313.4           Ch₃COCH₃         Ethyl acetate         178.0         5.205         521.3           n-C₀H₃         n-Pentane         244.2         5.784         341.           C(CH₃)₄         2,2-Dimethylpropane         340.9         6.464         193.           C₀H₀         Benzene         193.2         5.349         412.           C₀H₀         Benzene         193.2         5.349         412.           C₀H₁         PC₀H₁         n-Hexane         265.7         5.949         399.           Cl₂         Chlorine </th <th>CH₂CHCH₃</th> <th>Propylene</th> <th>129.2</th> <th>4.678</th> <th>298.9</th>	CH₂CHCH₃	Propylene	129.2	4.678	298.9
C₃H₀         Cyclopropane         140.2         4.807         248.5           C₃H₃         Propane         169.2         5.118         237.           n-C₃H₂OH         n-Propyl alcohol         118.8         4.549         576.           CH₃COOCH₃         Acetone         122.8         4.600         560.5           CH₃COOCH₃         Methyl acetate         151.8         4.936         469.3           n-C₄H₁₀         n-Butane         130.0         4.687         531.4           sio-C₄H₁₀         Isobutane         185.6         5.278         330.           C₃H₃OCH₃         Ethyl ether         231.0         5.678         313.4           Ch₃COCH₃         Ethyl acetate         178.0         5.205         521.3           n-C₀H₃         n-Pentane         244.2         5.784         341.           C(CH₃)₄         2,2-Dimethylpropane         340.9         6.464         193.           C₀H₀         Benzene         193.2         5.349         412.           C₀H₀         Benzene         193.2         5.349         412.           C₀H₁         PC₀H₁         n-Hexane         265.7         5.949         399.           Cl₂         Chlorine </td <td>CH₃CCH</td> <td>Methylacetylene</td> <td>136.2</td> <td>4.761</td> <td>251.8</td>	CH₃CCH	Methylacetylene	136.2	4.761	251.8
$n - C_3 H_7 OH$ $n - Propyl alcohol$ 118.8         4.549         576. $CH_5 COCH_5$ Acetone         122.8         4.600         560.5 $CH_5 COCH_5$ Methyl acetate         151.8         4.936         469.3 $n - C_4 H_{10}$ Isobutane         185.6         5.278         330. $c_2 H_5$ OC $c_2 H_5$ Ethyl ether         231.0         5.678         313.3 $C_2 H_5$ OC $c_2 H_5$ Ethyl acetate         178.0         5.205         521.3 $n - C_5 H_{12}$ $n - P$ entane         244.2         5.784         341. $C_6 CH_{12}$ $n - P$ entane         244.2         5.784         341. $C_6 H_6$ Benzene         193.2         5.349         412. $C_6 H_6$ Benzene         193.2         5.349         499.	$C_3H_6$		140.2	4.807	248.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_3H_8$	Propane	169.2	5.118	237.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	n-C <sub>3</sub> H <sub>7</sub> OH	n-Propyl alcohol	118.8	4.549	576.7
$n-C_4H_{10}$ $n$ -Butane         130.0         4.687         531.4           iso- $C_4H_{10}$ Isobutane         185.6         5.278         330. $C_9H_3CO_2H_5$ Ethyl ether         231.0         5.678         313.3 $CH_3COOC_2H_5$ Ethyl acetate         178.0         5.205         521.3 $n-C_5H_{12}$ $n$ -Pentane         244.2         5.784         341. $C(CH_3)_4$ 2,2-Dimethylpropane         340.9         6.464         193.2 $C_9H_0$ Benzene         193.2         5.349         412.3 $C_9H_0$ Benzene         298.2         6.182         297. $n$ - $C_9H_{14}$ $n$ -Hexane         265.7         5.949         399.3 $Cl_2$ Chlorine         94.65         4.217         316. $F_2$ Fluorine         47.75         3.357         112.4           HBr         Hydrogen bromide         47.58         3.353         449           HCN         Hydrogen chloride         46.98         3.339         344           HF         Hydrogen fluoride         39.37         3.148         330           H	CH <sub>3</sub> COCH <sub>3</sub>	3.15 E. SECTION CO.	122.8	4.600	560.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	CH₃COOCH₃	Methyl acetate	151.8	4.936	469.8
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	n-C <sub>4</sub> H <sub>10</sub>	n-Butane	130.0	4.687	531.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	iso -C4H10	Isobutane	185.6	5.278	330.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>2</sub> H <sub>5</sub> OC <sub>2</sub> H <sub>5</sub>	Ethyl ether	231.0	5.678	313.8
$n-C_5H_{12}$ $n$ -Pentane         244.2         5.784         341. $C(CH_3)_4$ 2,2-Dimethylpropane         340.9         6.464         193. $C_6H_6$ Benzene         193.2         5.349         412. $C_6H_{12}$ Cyclohexane         298.2         6.182         297. $n-C_6H_{14}$ $n$ -Hexane         265.7         5.949         399. $Cl_2$ Chlorine         94.65         4.217         316. $F_2$ Fluorine         47.75         3.357         112.           HBr         Hydrogen bromide         47.58         3.353         449           HCN         Hydrogen cyanide         60.37         3.630         569.           HCI         Hydrogen chloride         46.98         3.339         344.           HF         Hydrogen fluoride         39.37         3.148         330           HI         Hydrogen fluoride         94.24         4.211         288.           H <sub>2</sub> O         Water         23.25         2.641         809.           H <sub>2</sub> O         Water         23.25         2.641         809.           H <sub>2</sub> S         Hydrogen sulfide			178.0	5.205	521.3
$\begin{array}{c} C(CH_3)_4 \\ C_6H_6 \\ C_6H_6 \\ Benzene \\ C_6H_{12} \\ C_9C_1D_1 \\ C_2C_2C_1D_1 \\ C_3C_1C_2 \\ C_4C_1C_2C_2C_2C_2 \\ C_4C_1C_2C_2C_2C_2C_2 \\ C_4C_1C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2\\ C_4C_1C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C_2C$					341.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$					193.4
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$n-C_0H_{14}$ $n-Hexane$ $265.7$ $5.949$ $399.3$ $Cl_2$ Chlorine $94.65$ $4.217$ $316.1$ $F_2$ Fluorine $47.75$ $3.357$ $112.3$ HBr       Hydrogen bromide $47.58$ $3.357$ $412.3$ HBr       Hydrogen cyanide $60.37$ $3.630$ $569.5$ HCN       Hydrogen cyanide $60.37$ $3.630$ $569.5$ HCI       Hydrogen cyanide $40.98$ $3.339$ $344.5$ HCI       Hydrogen chloride $49.93.7$ $3.148$ $330$ HF       Hydrogen fluoride $39.37$ $3.148$ $330$ HI       Hydrogen iodide $94.24$ $4.211$ $288.5$ H <sub>2</sub> O       Water $23.25$ $2.641$ $809.5$ H <sub>2</sub> O       Water $23.24$ $4.196$ $289.5$ H <sub>2</sub> O       Hydrogen peroxide $93.24$ $4.196$ $289.5$ H <sub>2</sub> S       Hydrogen sulfide $60.02$ $3.623$ $301.5$ Hg       Mercury $33.03$ $2.969$ $750$			298.2	6.182	297.1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	B. 153				399.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$					316.0
HBr         Hydrogen bromide         47.58         3.353         449           HCN         Hydrogen cyanide         60.37         3.630         569.           HCl         Hydrogen chloride         46.98         3.339         344.           HF         Hydrogen fluoride         39.37         3.148         330           HI         Hydrogen iodide         94.24         4.211         288.           H2         Hydrogen         28.51         2.827         59.           H2O         Water         23.25         2.641         809.           H <sub>2</sub> O <sub>2</sub> Hydrogen peroxide         93.24         4.196         289.           H <sub>2</sub> S         Hydrogen sulfide         60.02         3.623         301.           Hg         Mercury         33.03         2.969         750           HgBr <sub>2</sub> Mercuric bromide         165.5         5.080         686.           HgCl <sub>2</sub> Mercuric chloride         118.9         4.550         750           HgI <sub>2</sub> Mercuric iodide         224.6         5.625         695.           I <sub>2</sub> Iodine         173.4         5.160         474.           NH <sub>3</sub> Ammonia         30.78			- Control of the Cont		112.6
HCN       Hydrogen cyanide       60.37       3.630       569.         HCl       Hydrogen chloride       46.98       3.339       344.         HF       Hydrogen fluoride       39.37       3.148       330         HI       Hydrogen iodide       94.24       4.211       288.         H2       Hydrogen       28.51       2.827       59.         H2O       Water       23.25       2.641       809.         H2O2       Hydrogen peroxide       93.24       4.196       289.         H2S       Hydrogen sulfide       60.02       3.623       301.         Hg       Mercury       33.03       2.969       750         HgBr2       Mercuric bromide       165.5       5.080       686.         HgCl2       Mercuric iodide       118.9       4.550       750         HgI2       Mercuric iodide       224.6       5.625       695.         I2       Iodine       173.4       5.160       474.         NH3       Ammonia       30.78       2.900       558.         NO       Nitric oxide       53.74       3.492       116.         NOCI       Nitrosyl chloride       87.75       4.112					
HCI       Hydrogen chloride       46.98       3.339       344.         HF       Hydrogen fluoride       39.37       3.148       330         HI       Hydrogen iodide       94.24       4.211       288.         H2       Hydrogen       28.51       2.827       59.         H2O       Water       23.25       2.641       809.         H2O2       Hydrogen peroxide       93.24       4.196       289.         H2S       Hydrogen sulfide       60.02       3.623       301.         Hg       Mercury       33.03       2.969       750         HgBr2       Mercuric bromide       165.5       5.080       686.         HgCl2       Mercuric chloride       118.9       4.550       750         HgI2       Mercuric iodide       224.6       5.625       695.         I2       Iodine       173.4       5.160       474.         NH3       Ammonia       30.78       2.900       558.         NO       Nitric oxide       53.74       3.492       116.         NOCI       Nitrosyl chloride       87.75       4.112       395.         N2       Nitrogen       69.14       3.798       71		, 0			569.1
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			94.24	4.211	288.7
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SiH <sub>4</sub> Silicon hydride 85.97 4.084 207.	100 100 <del>100 100 100 100 100 100 100 100</del>				171.9
	10000 to 2 000 Ext				207.6
511114 Statilite brothing 525.0 0.500 505.					563.7
UF <sub>6</sub> Uranium hexafluoride 268.1 5.967 236.		A			236.8

<sup>†</sup>R. A. Svehla, NASA Tech. Rep. R-132, Lewis Research Center, Cleveland, Ohio, 1962.  $b_0 = \frac{2}{3}\pi N_0 \sigma^3, \text{ where } N_0 \text{ is Avogadro's number.}$ 

<sup>§</sup>The parameter  $\sigma$  was determined by quantum-mechanical formulas.