Compounds considered for vapour pressure and heat of vaporization predictions

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Dipole | Compound | Dipole | Compound | Dipole |
| 1,3 butadiene | 0 | trichloroflouromethane | 0.45 | 1-propanol | 1.68 |
| anthracene | 0 | cis-2-butene | 0.5 | N,N Dimethyl aniline | 1.68 |
| argon | 0 | 2-methyl 1-butene | 0.51 | N-Methylaniline | 1.68 |
| benzene | 0 | indane | 0.54 | Ethanol | 1.68 |
| biphenyl | 0 | 1,7 Dimethylnaphthalene | 0.54 | chlorobenzene | 1.69 |
| decane | 0 | 1,2,3 trimethyl benzene | 0.56 | Methanol | 1.7 |
| fluorine | 0 | 1,2 Diethylbenzene (ortho) | 0.59 | acetic acid | 1.74 |
| naphthalene | 0 | trans 1,3 pentadiene | 0.68 | vinyl acetate | 1.79 |
| nonane | 0 | tertbutylbenzene | 0.7 | flouromethane | 1.85 |
| octo flouro cyclobutane | 0 | 1-pentyene | 0.81 | water | 1.85 |
| 2,2,3,3 Tetramethylbutane | 0 | diethyl amine | 0.92 | pyridine | 2.19 |
| 2,3,3 Trimethyl hexane | 0 | hydrogen sulfide | 0.97 | Dimethylethanoloamine | 2.21 |
| eicosane | 0 | hydrogen chloride | 1.08 | formaldehyde | 2.33 |
| butylcyclohexane | 0 | Diphenyl ether | 1.16 | pentane-2-one | 2.82 |
| Acetylene | 0 | 1 Bromonaphthalene | 1.29 | cyclopentanone | 2.93 |
| propylcyclopentane | 0 | dimethyl ether | 1.3 | nitromethane | 3.46 |
| nonadecane | 0 | 2-Heptanol | 1.34 | furfural | 3.6 |
| octadecane | 0 | phenol | 1.45 | acetonitrile | 3.92 |
| trans-2-butene | 0.3 | m-Toludiene | 1.49 | Propionitrile | 4.02 |
| hexafluorobenzene | 0.33 | dimethylsulfide | 1.5 | butyronitrile | 4.07 |
| 1-hexene | 0.34 | Methyl mercaptne | 1.52 |  |  |
| toluene | 0.36 | sulfur dioxide | 1.63 |  |  |
| butyl benzene | 0.37 | 1-hexanol | 1.65 |  |  |
| tri flouro chloroethylene | 0.4 | 1-Butanol | 1.66 |  |  |
| 1,2 Butadiene | 0.4 | Isopropanol | 1.66 |  |  |

Compounds considered for Second Virial Coefficients

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sr. No. | Compound | Dipole Moment | Temperature Range (K) |  |
| 1 | argon | 0 | 100-1000 |  |
| 2 | benzene | 0 | 290-600 |  |
| 3 | fluorine | 0 | 80-250 |  |
| 4 | hydrogen | 0 | 15-400 |  |
| 5 | naphthalene | 0 | 350-680 |  |
| 6 | acetylene | 0 | 199.63-273.15 |  |
| 7 | 1-hexene | 0.34 | 251.99-1511.94 |  |
| 8 | toluene | 0.36 | 350-430 |  |
| 9 | 1-decene | 0.42 | 308.2-1500 |  |
| 10 | trichloroflouromethane | 0.45 | 240-490 |  |
| 11 | hydrogen chloride | 1.08 | 190-470 |  |
| 12 | dimethyl ether | 1.3 | 275-310 |  |
| 13 | phenol | 1.45 | 478.15-623.15 |  |
| 14 | dimethylsulfide | 1.5 | 251.5-1509 |  |
| 15 | methyl mercaptne | 1.52 | 235-1410 |  |
| 16 | sulfur dioxide | 1.63 | 290-470 |  |
| 17 | 1-butanol | 1.66 | 350-440 |  |
| 18 | isopropanol | 1.66 | 279.58-2033.28 |  |
| 19 | 1-propanol | 1.68 | 380-430 |  |
| 20 | methanol | 1.7 | 320-420 |  |
| 21 | water | 1.85 | 300-1200 |  |
| 22 | pyridine | 2.19 | 340-440 |  |
| 23 | ethylene glycol | 2.31 | 323-3223 |  |
| 24 | formaldehyde | 2.33 | 201-2034 |  |
| 25 | pentane-2-one | 2.82 | 330-400 |  |

Compounds considered for Saturated Liquid Density

|  |  |  |  |
| --- | --- | --- | --- |
| Sr. No. | Compound | Dipole Moment | Temperature Range (K) |
| 1 | 1,3 butadiene | 0 | 165-424 |
| 2 | benzene | 0 | 273-561 |
| 3 | naphthalene | 0 | 373-548 |
| 4 | 1-hexene | 0.34 | 146-325 |
| 5 | n-butanol | 1.66 | 213-558 |
| 6 | 1-propanol | 1.68 | 186-507 |
| 7 | ethanol | 1.69 | 191-513 |
| 8 | ethyl acetate | 1.75 | 294-280 |
| 9 | Water | 1.85 | 273-648 |
| 10 | NMP | 4.1 | 253-363 |