# 1,3-Butanediol

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|---|---|
| **Other names:** | «beta»-Butylene glycol |
| | Methyltrimethylene glycol |
| | 1-Methyl-1,3-propanediol |
| | 1,3-Butylene glycol |
| | 1,3-Dihydroxybutane |
| | Butane-1,3-diol |
| | BD |
| | 1,3-Butandiol |
| | 1,3-Butylenglykol |
| | 1,3-Butanodiol |
| | Butanediol,1,3- |
| | (RS)-1,3-Butanediol |
| | Butylene glycol |
| | NSC 402145 |
| | 1,3-butanediol, DL- |
| **Inchi:** | InChI=1S/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3 |
| **InchiKey:** | PUPZLCDOIYMWBV-UHFFFAOYSA-N |
| **Formula:** | C4H10O2 |
| **SMILES:** | CC(O)CCO |
| **Mol. weight [g/mol]:** | 90.12 |
| **CAS:** | 18826-95-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -293.28 | kJ/mol | Joback Method |
| hf | -435.63 | kJ/mol | Joback Method |
| hfus | 10.77 | kJ/mol | Joback Method |
| hvap | 57.47 | kJ/mol | Joback Method |
| log10ws | -0.14 | | Crippen Method |
| logp | -0.250 | | Crippen Method |
| mcvol | 78.960 | ml/mol | McGowan Method |
| pc | 4020.00 ± 250.00 | kPa | NIST Webbook |
| rhoc | 294.79 ± 11.72 | kg/m3 | NIST Webbook |
| tb | 474.84 | K | Joback Method |
| tc | 676.00 ± 2.00 | K | NIST Webbook |
| tf | 241.48 | K | Joback Method |
| vc | 0.291 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 173.31 | J/mol×K | 474.84 | Joback Method |
| cpg | 179.93 | J/mol×K | 501.78 | Joback Method |
| cpg | 186.29 | J/mol×K | 528.72 | Joback Method |
| cpg | 192.41 | J/mol×K | 555.66 | Joback Method |
| cpg | 198.29 | J/mol×K | 582.59 | Joback Method |
| cpg | 203.94 | J/mol×K | 609.53 | Joback Method |
| cpg | 209.35 | J/mol×K | 636.47 | Joback Method |
| dvisc | 0.6060212 | Pa×s | 241.48 | Joback Method |
| dvisc | 0.0554139 | Pa×s | 280.37 | Joback Method |
| dvisc | 0.0090753 | Pa×s | 319.27 | Joback Method |
| dvisc | 0.0022017 | Pa×s | 358.16 | Joback Method |
| dvisc | 0.0007050 | Pa×s | 397.05 | Joback Method |
| dvisc | 0.0002766 | Pa×s | 435.95 | Joback Method |
| dvisc | 0.0001265 | Pa×s | 474.84 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C18826954&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rhoc:** | Critical density |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |