# 1,3-Butanediol, (S)-

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|---|---|
| **Other names:** | (+)-1,3-Butanediol |
| | (S)-(+)-1,3-Butanediol |
| | (S)-(+)-butane-1,3-diol |
| | D-Butane-1,3-diol |
| **Inchi:** | InChI=1S/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3/t4-/m1/s1 |
| **InchiKey:** | PUPZLCDOIYMWBV-SCSAIBSYSA-N |
| **Formula:** | C4H10O2 |
| **SMILES:** | CC(O)CCO |
| **Mol. weight [g/mol]:** | 90.12 |
| **CAS:** | 24621-61-2 |

## 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 | 5029.93 | kPa | Joback Method |
| tb | 474.84 | K | Joback Method |
| tc | 636.47 | K | Joback Method |
| 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 | 203.94 | J/mol×K | 609.53 | Joback Method |
| cpg | 198.29 | J/mol×K | 582.59 | Joback Method |
| cpg | 192.41 | J/mol×K | 555.66 | Joback Method |
| cpg | 186.29 | J/mol×K | 528.72 | Joback Method |

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|---|---|---|---|---|
| cpg | 179.93 | J/mol×K | 501.78 | Joback Method |
| cpg | 209.35 | J/mol×K | 636.47 | Joback Method |
| dvisc | 0.0001265 | Pa×s | 474.84 | Joback Method |
| dvisc | 0.0002766 | Pa×s | 435.95 | Joback Method |
| dvisc | 0.0007050 | Pa×s | 397.05 | Joback Method |
| dvisc | 0.0022017 | Pa×s | 358.16 | Joback Method |
| dvisc | 0.0090753 | Pa×s | 319.27 | Joback Method |
| dvisc | 0.0554139 | Pa×s | 280.37 | Joback Method |
| dvisc | 0.6060212 | Pa×s | 241.48 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 382.20 | K | 1.90 | NIST Webbook |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C24621612&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |

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|---|---|
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |