# 1,2-Cyclohexanediol, trans-

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|---|---|
| **Other names:** | (1R,2R)-1,2-cyclohexanediol |
| | 1,2-Cyclohexanediol, (E)- |
| | 1,2-trans-Cyclohexanediol |
| | trans-1,2-Cyclohexanediol |
| | trans-1,2-Dihydroxycyclohexane |
| | trans-cyclohexane-1,2-diol |
| **Inchi:** | InChI=1S/C6H12O2/c7-5-3-1-2-4-6(5)8/h5-8H,1-4H2/t5-,6-/m1/s1 |
| **InchiKey:** | PFURGBBHAOXLIO-PHDIDXHHSA-N |
| **Formula:** | C6H12O2 |
| **SMILES:** | OC1CCCCC1O |
| **Mol. weight [g/mol]:** | 116.16 |
| **CAS:** | 1460-57-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3520.00 ± 0.80 | kJ/mol | NIST Webbook |
| gf | -257.26 | kJ/mol | Joback Method |
| hf | -437.65 | kJ/mol | Joback Method |
| hfus | 12.38 | kJ/mol | Joback Method |
| hvap | 62.43 | kJ/mol | Joback Method |
| log10ws | -0.98 | | Crippen Method |
| logp | 0.282 | | Crippen Method |
| mcvol | 96.280 | ml/mol | McGowan Method |
| pc | 4835.95 | kPa | Joback Method |
| tb | 535.92 | K | Joback Method |
| tc | 720.36 | K | Joback Method |
| tf | 376.40 | K | Solid-Liquid Equilibria of the trans-1,2-Cyclohexanediol + Ethyl Acetate + Water Ternary System |
| tf | 376.65 ± 1.50 | K | NIST Webbook |
| tf | 381.00 | K | A Novel Co-crystal of (R,R)-1,2-Cyclohexanediol with (R,R)-Tartaric Acid, a Key Structure for Resolution of the Racemic (+-)-trans-Diol in Supercritical Carbon Dioxide, and the Binary Melting Phase Relations. |

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|---|---|---|---|
| vc | 0.342 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 241.23 | J/mol×K | 535.92 | Joback Method |
| cpg | 252.43 | J/mol×K | 566.66 | Joback Method |
| cpg | 263.09 | J/mol×K | 597.40 | Joback Method |
| cpg | 273.22 | J/mol×K | 628.14 | Joback Method |
| cpg | 282.84 | J/mol×K | 658.88 | Joback Method |
| cpg | 291.95 | J/mol×K | 689.62 | Joback Method |
| cpg | 300.56 | J/mol×K | 720.36 | Joback Method |
| dvisc | 0.0000802 | Pa×s | 535.92 | Joback Method |
| dvisc | 0.0131225 | Pa×s | 324.45 | Joback Method |
| dvisc | 0.0029585 | Pa×s | 366.75 | Joback Method |
| dvisc | 0.0909733 | Pa×s | 282.16 | Joback Method |
| dvisc | 0.0003475 | Pa×s | 451.33 | Joback Method |
| dvisc | 0.0001568 | Pa×s | 493.63 | Joback Method |
| dvisc | 0.0009076 | Pa×s | 409.04 | Joback Method |
| hfust | 21.00 | kJ/mol | 382.60 | NIST Webbook |
| hfust | 16.37 | kJ/mol | 375.70 | NIST Webbook |
| hfust | 18.51 | kJ/mol | 372.30 | NIST Webbook |
| hfust | 18.51 | kJ/mol | 372.30 | NIST Webbook |
| hsubt | 85.90 ± 1.40 | kJ/mol | 343.00 | NIST Webbook |
| hsubt | 42.50 | kJ/mol | 304.50 | NIST Webbook |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **A Novel Co-crystal of (R,R)-1,2-Cyclohexanediol with (R,R)-Tartaric Acid, a Key Structure for Resolution of the Racemic trans-1,2-Cyclohexanediol + Ethyl Acetate System:** | https://www.doi.org/10.1016/j.tca.2009.09.001 |
| **Solid-Liquid Equilibria of the (+)-trans-Diol in Supercritical Carbon Dioxide, and the Binary Melting Phase Relations.:** | https://www.doi.org/10.1021/je050338e |
| **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=C1460577&Units=SI |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |