# 2,2,5,5-Tetramethylhexan-3-ol

**Inchi:** InChI=1S/C10H22O/c1-9(2,3)7-8(11)10(4,5)6/h8,11H,7H2,1-6H3
**InchiKey:** CFEYPBVKHMZCFR-UHFFFAOYSA-N
**Formula:** C10H22O
**SMILES:** CC(C)(C)CC(O)C(C)(C)C
**Mol. weight [g/mol]:** 158.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5581 | | Cheméo Relay (1.0) |
| gf | -100.26 | kJ/mol | Joback Method |
| hf | -424.12 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 7.39 | kJ/mol | Joback Method |
| hvap | 64.88 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.58 | eV | Cheméo Relay (1.0) |
| log10ws | -2.79 | | Cheméo Relay (1.0) |
| logp | 2.830 | | Crippen Method |
| mcvol | 157.630 | ml/mol | McGowan Method |
| pc | 2402.92 | kPa | Joback Method |
| tb | 443.15 ± 5.00 | K | NIST Webbook |
| tb | 446.65 ± 4.00 | K | NIST Webbook |
| tc | 646.71 | K | Cheméo Relay (1.0) |
| tf | 334.06 | K | Cheméo Relay (1.0) |
| vc | 0.579 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 386.67 | J/mol×K | 513.48 | Joback Method |
| cpg | 467.33 | J/mol×K | 692.84 | Joback Method |
| cpg | 455.72 | J/mol×K | 662.94 | Joback Method |
| cpg | 443.43 | J/mol×K | 633.05 | Joback Method |
| cpg | 430.42 | J/mol×K | 603.16 | Joback Method |
| cpg | 416.65 | J/mol×K | 573.27 | Joback Method |
| cpg | 402.08 | J/mol×K | 543.37 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0011137 | Pa×s | 383.30 | Joback Method |
| dvisc | 0.0001107 | Pa×s | 513.48 | Joback Method |
| dvisc | 0.0002073 | Pa×s | 470.09 | Joback Method |
| dvisc | 0.0004411 | Pa×s | 426.69 | Joback Method |
| dvisc | 0.1204426 | Pa×s | 253.12 | Joback Method |
| dvisc | 0.0035617 | Pa×s | 339.91 | Joback Method |
| dvisc | 0.0160077 | Pa×s | 296.51 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C55073864&Units=SI |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **ie:** | Ionization energy |
| **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 |

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