# 1-Octanol, 3,7-dimethyl-, (S)-

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|---|---|
| **Other names:** | (-)-3,7-Dimethyl-1-octanol |
| | (S)-3,7-Dimethyl-1-octanol |
| | (S)-Dihydrocitronellol |
| **Inchi:** | InChI=1S/C10H22O/c1-9(2)5-4-6-10(3)7-8-11/h9-11H,4-8H2,1-3H3/t10-/m1/s1 |
| **InchiKey:** | PRNCMAKCNVRZFX-SNVBAGLBSA-N |
| **Formula:** | C10H22O |
| **SMILES:** | CC(C)CCCC(C)CCO |
| **Mol. weight [g/mol]:** | 158.28 |
| **CAS:** | 68680-98-8 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -108.38 | kJ/mol | Joback Method |
| hf | -412.52 | kJ/mol | Joback Method |
| hfus | 18.70 | kJ/mol | Joback Method |
| hvap | 53.76 | kJ/mol | Joback Method |
| log10ws | -2.79 | | Crippen Method |
| logp | 2.831 | | Crippen Method |
| mcvol | 157.630 | ml/mol | McGowan Method |
| pc | 2333.78 | kPa | Joback Method |
| tb | 519.50 | K | Joback Method |
| tc | 683.75 | K | Joback Method |
| tf | 233.28 | K | Joback Method |
| vc | 0.603 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 381.07 | J/mol×K | 519.50 | Joback Method |
| cpg | 394.90 | J/mol×K | 546.87 | Joback Method |
| cpg | 408.18 | J/mol×K | 574.25 | Joback Method |
| cpg | 420.93 | J/mol×K | 601.62 | Joback Method |
| cpg | 433.16 | J/mol×K | 629.00 | Joback Method |
| cpg | 444.88 | J/mol×K | 656.37 | Joback Method |

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|---|---|---|---|---|
| cpg | 456.11 | J/mol×K | 683.75 | Joback Method |
| dvisc | 0.1480969 | Pa×s | 233.28 | Joback Method |
| dvisc | 0.0161218 | Pa×s | 280.98 | Joback Method |
| dvisc | 0.0033408 | Pa×s | 328.69 | Joback Method |
| dvisc | 0.0010317 | Pa×s | 376.39 | Joback Method |
| dvisc | 0.0004150 | Pa×s | 424.09 | Joback Method |
| dvisc | 0.0002007 | Pa×s | 471.80 | Joback Method |
| dvisc | 0.0001109 | Pa×s | 519.50 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 378.50 ± 0.50 | K | 2.00 | NIST Webbook |

# Sources

**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=C68680988&Units=SI
**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
**pc:** Critical Pressure
**tb:** Normal Boiling Point Temperature

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