# Neo iso-verbanol

**Inchi:** InChI=1S/C10H18O/c1-6-4-9(11)8-5-7(6)10(8,2)3/h6-9,11H,4-5H2,1-3H3
**InchiKey:** VIGNRSKBPLHDGV-UHFFFAOYSA-N
**Formula:** C10H18O
**SMILES:** CC1CC(O)C2CC1C2(C)C
**Mol. weight [g/mol]:** 154.25
**CAS:** 94480-81-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -22.72 | kJ/mol | Joback Method |
| hf | -308.30 | kJ/mol | Joback Method |
| hfus | 16.83 | kJ/mol | Joback Method |
| hvap | 52.45 | kJ/mol | Joback Method |
| log10ws | -2.21 | | Crippen Method |
| logp | 2.049 | | Crippen Method |
| mcvol | 135.910 | ml/mol | McGowan Method |
| pc | 2906.11 | kPa | Joback Method |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| tb | 524.36 | K | Joback Method |
| tc | 717.42 | K | Joback Method |
| tf | 306.82 | K | Joback Method |
| vc | 0.515 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 355.48 | J/mol×K | 524.36 | Joback Method |
| cpg | 372.00 | J/mol×K | 556.54 | Joback Method |
| cpg | 387.53 | J/mol×K | 588.71 | Joback Method |
| cpg | 402.17 | J/mol×K | 620.89 | Joback Method |
| cpg | 416.03 | J/mol×K | 653.07 | Joback Method |
| cpg | 429.20 | J/mol×K | 685.24 | Joback Method |

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|---|---|---|---|---|
| cpg | 441.78 | J/mol×K | 717.42 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C94480816&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |