# «beta»-Cyclolavandulal

**Inchi:** InChI=1S/C10H16O/c1-8-6-10(2,3)5-4-9(8)7-11/h7H,4-6H2,1-3H3
**InchiKey:** OHCMANJUZNNOQW-UHFFFAOYSA-N
**Formula:** C10H16O
**SMILES:** CC1=C(C=O)CCC(C)(C)C1
**Mol. weight [g/mol]:** 152.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -36.54 | kJ/mol | Joback Method |
| hf | -230.91 | kJ/mol | Joback Method |
| hfus | 9.93 | kJ/mol | Joback Method |
| hvap | 45.47 | kJ/mol | Joback Method |
| log10ws | -2.80 | | Crippen Method |
| logp | 2.712 | | Crippen Method |
| mcvol | 138.170 | ml/mol | McGowan Method |
| pc | 2928.17 | kPa | Joback Method |
| rinpol | 1207.00 | | NIST Webbook |
| rinpol | 1207.00 | | NIST Webbook |
| ripol | 1656.00 | | NIST Webbook |
| tb | 505.77 | K | Joback Method |
| tc | 720.94 | K | Joback Method |
| tf | 301.54 | K | Joback Method |
| vc | 0.529 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 313.28 | J/mol×K | 505.77 | Joback Method |
| cpg | 329.19 | J/mol×K | 541.63 | Joback Method |
| cpg | 344.11 | J/mol×K | 577.49 | Joback Method |
| cpg | 358.15 | J/mol×K | 613.35 | Joback Method |
| cpg | 371.41 | J/mol×K | 649.21 | Joback Method |
| cpg | 383.99 | J/mol×K | 685.08 | Joback Method |
| cpg | 396.00 | J/mol×K | 720.94 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R418794&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

| | |
|---|---|
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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