# «beta»-Cyclolavandulyl propionate

**Inchi:** InChI=1S/C13H22O2/c1-5-12(14)15-9-11-6-7-13(3,4)8-10(11)2/h5-9H2,1-4H3
**InchiKey:** FYFSCEZHVSYIGI-UHFFFAOYSA-N
**Formula:** C13H22O2
**SMILES:** CCC(=O)OCC1=C(C)CC(C)(C)CC1
**Mol. weight [g/mol]:** 210.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -145.68 | kJ/mol | Joback Method |
| hf | -452.05 | kJ/mol | Joback Method |
| hfus | 18.19 | kJ/mol | Joback Method |
| hvap | 54.58 | kJ/mol | Joback Method |
| log10ws | -3.63 | | Crippen Method |
| logp | 3.466 | | Crippen Method |
| mcvol | 186.310 | ml/mol | McGowan Method |
| pc | 2135.43 | kPa | Joback Method |
| rinpol | 1391.00 | | NIST Webbook |
| ripol | 1712.00 | | NIST Webbook |
| tb | 602.04 | K | Joback Method |
| tc | 809.71 | K | Joback Method |
| tf | 365.51 | K | Joback Method |
| vc | 0.705 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 484.22 | J/mol×K | 602.04 | Joback Method |
| cpg | 502.08 | J/mol×K | 636.65 | Joback Method |
| cpg | 519.05 | J/mol×K | 671.26 | Joback Method |
| cpg | 535.23 | J/mol×K | 705.87 | Joback Method |
| cpg | 550.69 | J/mol×K | 740.48 | Joback Method |
| cpg | 565.53 | J/mol×K | 775.10 | Joback Method |
| cpg | 579.83 | J/mol×K | 809.71 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R418843&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 |