# «beta»-Cyclolavandulyl isobutyrate

**Inchi:** InChI=1S/C14H24O2/c1-10(2)13(15)16-9-12-6-7-14(4,5)8-11(12)3/h10H,6-9H2,1-5H3
**InchiKey:** MPXQTTNSJUOAST-UHFFFAOYSA-N
**Formula:** C14H24O2
**SMILES:** CC1=C(COC(=O)C(C)C)CCC(C)(C)C1
**Mol. weight [g/mol]:** 224.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -139.70 | kJ/mol | Joback Method |
| hf | -477.97 | kJ/mol | Joback Method |
| hfus | 17.26 | kJ/mol | Joback Method |
| hvap | 56.42 | kJ/mol | Joback Method |
| log10ws | -3.81 | | Crippen Method |
| logp | 3.712 | | Crippen Method |
| mcvol | 200.400 | ml/mol | McGowan Method |
| pc | 1971.80 | kPa | Joback Method |
| rinpol | 1432.00 | | NIST Webbook |
| rinpol | 1432.00 | | NIST Webbook |
| ripol | 1702.00 | | NIST Webbook |
| ripol | 1702.00 | | NIST Webbook |
| tb | 624.48 | K | Joback Method |
| tc | 833.00 | K | Joback Method |
| tf | 361.78 | K | Joback Method |
| vc | 0.754 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 536.65 | J/mol×K | 624.48 | Joback Method |
| cpg | 555.42 | J/mol×K | 659.23 | Joback Method |
| cpg | 573.27 | J/mol×K | 693.99 | Joback Method |
| cpg | 590.29 | J/mol×K | 728.74 | Joback Method |
| cpg | 606.58 | J/mol×K | 763.50 | Joback Method |
| cpg | 622.21 | J/mol×K | 798.25 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 637.28 | J/mol×K | 833.00 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R418823&Units=SI |

# 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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