# Isoverbanol, acetate

**Inchi:** InChI=1S/C12H20O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h7,9-11H,5-6H2,1-4H3
**InchiKey:** SJTUFGGNSOBUCB-UHFFFAOYSA-N
**Formula:** C12H20O2
**SMILES:** CC(=O)OC1CC(C)C2CC1C2(C)C
**Mol. weight [g/mol]:** 196.29

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -102.98 | kJ/mol | Joback Method |
| hf | -442.15 | kJ/mol | Joback Method |
| hfus | 20.71 | kJ/mol | Joback Method |
| hvap | 49.38 | kJ/mol | Joback Method |
| log10ws | -2.64 | | Crippen Method |
| logp | 2.620 | | Crippen Method |
| mcvol | 165.660 | ml/mol | McGowan Method |
| pc | 2282.77 | kPa | Joback Method |
| rinpol | 1310.00 | | NIST Webbook |
| rinpol | 1296.00 | | NIST Webbook |
| rinpol | 1296.00 | | NIST Webbook |
| rinpol | 1296.00 | | NIST Webbook |
| tb | 554.23 | K | Joback Method |
| tc | 761.49 | K | Joback Method |
| tf | 340.70 | K | Joback Method |
| vc | 0.632 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 439.79 | J/mol×K | 554.23 | Joback Method |
| cpg | 459.08 | J/mol×K | 588.77 | Joback Method |
| cpg | 477.26 | J/mol×K | 623.32 | Joback Method |
| cpg | 494.44 | J/mol×K | 657.86 | Joback Method |
| cpg | 510.73 | J/mol×K | 692.40 | Joback Method |
| cpg | 526.25 | J/mol×K | 726.95 | Joback Method |

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|---|---|---|---|---|
| cpg | 541.10 | J/mol×K | 761.49 | Joback Method |

# Sources

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|---|---|
| **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=R130053&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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