# neo-iso-Verbenol acetate

**Inchi:** InChI=1S/C12H18O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h5,9-11H,6H2,1-4H3/t9-,1
**InchiKey:** OZBFUQLOVFXDNK-AXFHLTTASA-N
**Formula:** C12H18O2
**SMILES:** CC(=O)OC1C=C(C)C2CC1C2(C)C
**Mol. weight [g/mol]:** 194.27
**CAS:** 73366-12-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -74.94 | kJ/mol | Joback Method |
| hf | -375.50 | kJ/mol | Joback Method |
| hfus | 20.47 | kJ/mol | Joback Method |
| hvap | 50.64 | kJ/mol | Joback Method |
| log10ws | -2.74 | | Crippen Method |
| logp | 2.540 | | Crippen Method |
| mcvol | 161.360 | ml/mol | McGowan Method |
| pc | 2405.28 | kPa | Joback Method |
| rinpol | 1328.00 | | NIST Webbook |
| rinpol | 1328.00 | | NIST Webbook |
| tb | 563.04 | K | Joback Method |
| tc | 773.40 | K | Joback Method |
| tf | 358.22 | K | Joback Method |
| vc | 0.620 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.92 | J/mol×K | 563.04 | Joback Method |
| cpg | 437.32 | J/mol×K | 598.10 | Joback Method |
| cpg | 453.71 | J/mol×K | 633.16 | Joback Method |
| cpg | 469.20 | J/mol×K | 668.22 | Joback Method |
| cpg | 483.90 | J/mol×K | 703.28 | Joback Method |
| cpg | 497.94 | J/mol×K | 738.34 | Joback Method |
| cpg | 511.43 | J/mol×K | 773.40 | 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=C73366128&Units=SI |

# 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 |