# Neopentyl (E)-2-methylbut-2-enoate

**Inchi:** InChI=1S/C10H18O2/c1-6-8(2)9(11)12-7-10(3,4)5/h6H,7H2,1-5H3/b8-6+
**InchiKey:** CBFZVDUBQXGOSX-SOFGYWHQSA-N
**Formula:** C10H18O2
**SMILES:** CC=C(C)C(=O)OCC(C)(C)C
**Mol. weight [g/mol]:** 170.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -126.09 | kJ/mol | Joback Method |
| hf | -395.85 | kJ/mol | Joback Method |
| hfus | 15.92 | kJ/mol | Joback Method |
| hvap | 45.75 | kJ/mol | Joback Method |
| log10ws | -2.48 | | Crippen Method |
| logp | 2.542 | | Crippen Method |
| mcvol | 154.900 | ml/mol | McGowan Method |
| pc | 2365.67 | kPa | Joback Method |
| rinpol | 1128.00 | | NIST Webbook |
| tb | 505.30 | K | Joback Method |
| tc | 699.32 | K | Joback Method |
| tf | 258.00 | K | Joback Method |
| vc | 0.590 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 353.60 | J/mol×K | 505.30 | Joback Method |
| cpg | 368.69 | J/mol×K | 537.64 | Joback Method |
| cpg | 382.99 | J/mol×K | 569.97 | Joback Method |
| cpg | 396.52 | J/mol×K | 602.31 | Joback Method |
| cpg | 409.32 | J/mol×K | 634.65 | Joback Method |
| cpg | 421.42 | J/mol×K | 666.98 | Joback Method |
| cpg | 432.86 | J/mol×K | 699.32 | 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=U373710&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 |