# Acetic acid, iso-butenyl ester

**Inchi:** InChI=1S/C6H10O2/c1-5(2)4-8-6(3)7/h4H,1-3H3
**InchiKey:** MNJRLZXXSZEIHD-UHFFFAOYSA-N
**Formula:** C6H10O2
**SMILES:** CC(=O)OC=C(C)C
**Mol. weight [g/mol]:** 114.14
**CAS:** 14478-14-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -162.61 | kJ/mol | Joback Method |
| hf | -304.54 | kJ/mol | Joback Method |
| hfus | 12.97 | kJ/mol | Joback Method |
| hvap | 38.14 | kJ/mol | Joback Method |
| log10ws | -1.55 | | Crippen Method |
| logp | 1.473 | | Crippen Method |
| mcvol | 98.540 | ml/mol | McGowan Method |
| pc | 3497.14 | kPa | Joback Method |
| tb | 417.01 | K | Joback Method |
| tc | 607.33 | K | Joback Method |
| tf | 210.50 | K | Joback Method |
| vc | 0.377 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 184.26 | J/mol×K | 417.01 | Joback Method |
| cpg | 193.90 | J/mol×K | 448.73 | Joback Method |
| cpg | 203.14 | J/mol×K | 480.45 | Joback Method |
| cpg | 212.00 | J/mol×K | 512.17 | Joback Method |
| cpg | 220.47 | J/mol×K | 543.89 | Joback Method |
| cpg | 228.57 | J/mol×K | 575.61 | Joback Method |
| cpg | 236.31 | J/mol×K | 607.33 | 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=C14478149&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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