# Acetoacetic acid isoamyl ester

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|---|---|
| **Other names:** | Butanoic acid, 3-oxo-, 3-methylbutyl ester |
| | Isoamyl acetoacetate |
| | 3-Methylbutyl 3-oxobutanoate |
| | Isoamyl acetylacetate |
| | Isoamyl «beta»-ketobutyrate |
| | Isopentyl «beta»-ketobutyrate |
| | isopentyl acetoacetate |
| **Inchi:** | InChI=1S/C9H16O3/c1-7(2)4-5-12-9(11)6-8(3)10/h7H,4-6H2,1-3H3 |
| **InchiKey:** | XHRGPLDMNNGHCX-UHFFFAOYSA-N |
| **Formula:** | C9H16O3 |
| **SMILES:** | CC(=O)CC(=O)OCCC(C)C |
| **Mol. weight [g/mol]:** | 172.22 |
| **CAS:** | 2308-18-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -340.38 | kJ/mol | Joback Method |
| hf | -591.75 | kJ/mol | Joback Method |
| hfus | 19.93 | kJ/mol | Joback Method |
| hvap | 51.14 | kJ/mol | Joback Method |
| log10ws | -1.49 | | Crippen Method |
| logp | 1.555 | | Crippen Method |
| mcvol | 146.680 | ml/mol | McGowan Method |
| pc | 2589.85 | kPa | Joback Method |
| tb | 491.00 | K | NIST Webbook |
| tc | 721.50 | K | Joback Method |
| tf | 298.28 | K | Joback Method |
| vc | 0.564 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 343.82 | J/mol×K | 535.04 | Joback Method |
| cpg | 356.65 | J/mol×K | 566.12 | Joback Method |

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|---|---|---|---|---|
| cpg | 368.94 | J/mol×K | 597.19 | Joback Method |
| cpg | 380.69 | J/mol×K | 628.27 | Joback Method |
| cpg | 391.90 | J/mol×K | 659.35 | Joback Method |
| cpg | 402.58 | J/mol×K | 690.42 | Joback Method |
| cpg | 412.73 | J/mol×K | 721.50 | Joback Method |
| dvisc | 0.0035617 | Pa×s | 298.28 | Joback Method |
| dvisc | 0.0017528 | Pa×s | 337.74 | Joback Method |
| dvisc | 0.0010005 | Pa×s | 377.20 | Joback Method |
| dvisc | 0.0006351 | Pa×s | 416.66 | Joback Method |
| dvisc | 0.0004361 | Pa×s | 456.12 | Joback Method |
| dvisc | 0.0003180 | Pa×s | 495.58 | Joback Method |
| dvisc | 0.0002429 | Pa×s | 535.04 | Joback Method |

# Sources

**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=C2308181&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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