# Propanedioic acid, acetyl-, diethyl ester

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|---|---|
| **Other names:** | Malonic acid, acetyl-, diethyl ester |
| | C-Acetylmalonic ester |
| | Diethyl acetylmalonate |
| | Ethyl acetomalonate |
| | Diethyl 2-acetylmalonate |
| | Ethyl acetylmalonate |
| | Diethyl acetomalonate |
| **Inchi:** | InChI=1S/C9H14O5/c1-4-13-8(11)7(6(3)10)9(12)14-5-2/h7H,4-5H2,1-3H3 |
| **InchiKey:** | SQAUUQRBOCJRCW-UHFFFAOYSA-N |
| **Formula:** | C9H14O5 |
| **SMILES:** | CCOC(=O)C(C(C)=O)C(=O)OCC |
| **Mol. weight [g/mol]:** | 202.20 |
| **CAS:** | 570-08-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -574.30 | kJ/mol | Joback Method |
| hf | -836.55 | kJ/mol | Joback Method |
| hfus | 22.72 | kJ/mol | Joback Method |
| hvap | 60.30 | kJ/mol | Joback Method |
| log10ws | -0.35 | | Crippen Method |
| logp | 0.318 | | Crippen Method |
| mcvol | 154.120 | ml/mol | McGowan Method |
| pc | 2715.50 | kPa | Joback Method |
| tb | 611.33 | K | Joback Method |
| tc | 804.41 | K | Joback Method |
| tf | 370.44 | K | Joback Method |
| vc | 0.588 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 385.35 | J/mol×K | 611.33 | Joback Method |
| cpg | 397.13 | J/mol×K | 643.51 | Joback Method |

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|---|---|---|---|---|
| cpg | 408.34 | J/mol×K | 675.69 | Joback Method |
| cpg | 418.99 | J/mol×K | 707.87 | Joback Method |
| cpg | 429.06 | J/mol×K | 740.05 | Joback Method |
| cpg | 438.55 | J/mol×K | 772.23 | Joback Method |
| cpg | 447.44 | J/mol×K | 804.41 | Joback Method |
| dvisc | 0.0020254 | Pa×s | 370.44 | Joback Method |
| dvisc | 0.0011397 | Pa×s | 410.59 | Joback Method |
| dvisc | 0.0007104 | Pa×s | 450.74 | Joback Method |
| dvisc | 0.0004785 | Pa×s | 490.88 | Joback Method |
| dvisc | 0.0003421 | Pa×s | 531.03 | Joback Method |
| dvisc | 0.0002564 | Pa×s | 571.18 | Joback Method |
| dvisc | 0.0001996 | Pa×s | 611.33 | Joback Method |
| hvapt | 54.00 | kJ/mol | 436.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 398.00 | K | 2.70 | NIST Webbook |

# 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=C570081&Units=SI

# 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

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| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |