# Acetoxyacetic acid, 2-(1-adamantyl)ethyl ester

**Inchi:** InChI=1S/C16H24O4/c1-11(17)20-10-15(18)19-3-2-16-7-12-4-13(8-16)6-14(5-12)9-16/h1
**InchiKey:** ANKZCVBEWNJHPO-UHFFFAOYSA-N
**Formula:** C16H24O4
**SMILES:** CC(=O)OCC(=O)OCCC12CC3CC(CC(C3)C1)C2
**Mol. weight [g/mol]:** 280.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -227.05 | kJ/mol | Joback Method |
| hf | -656.03 | kJ/mol | Joback Method |
| hfus | 29.85 | kJ/mol | Joback Method |
| hvap | 67.97 | kJ/mol | Joback Method |
| log10ws | -2.96 | | Crippen Method |
| logp | 2.699 | | Crippen Method |
| mcvol | 218.600 | ml/mol | McGowan Method |
| pc | 2001.91 | kPa | Joback Method |
| rinpol | 2009.00 | | NIST Webbook |
| tb | 738.12 | K | Joback Method |
| tc | 950.84 | K | Joback Method |
| tf | 484.36 | K | Joback Method |
| vc | 0.840 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 689.70 | J/mol×K | 738.12 | Joback Method |
| cpg | 708.23 | J/mol×K | 773.57 | Joback Method |
| cpg | 725.98 | J/mol×K | 809.03 | Joback Method |
| cpg | 743.10 | J/mol×K | 844.48 | Joback Method |
| cpg | 759.76 | J/mol×K | 879.93 | Joback Method |
| cpg | 776.10 | J/mol×K | 915.38 | Joback Method |
| cpg | 792.30 | J/mol×K | 950.84 | Joback Method |

# Sources

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|---|---|
| **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=U308317&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 |