# Adamantan-4-one, 1-methoxy

**Inchi:** InChI=1S/C11H16O2/c1-13-11-4-7-2-8(5-11)10(12)9(3-7)6-11/h7-9H,2-6H2,1H3
**InchiKey:** PKPPAWGCOMEBLA-UHFFFAOYSA-N
**Formula:** C11H16O2
**SMILES:** COC12CC3CC(C1)C(=O)C(C3)C2
**Mol. weight [g/mol]:** 180.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -28.90 | kJ/mol | Joback Method |
| hf | -333.15 | kJ/mol | Joback Method |
| hfus | 12.02 | kJ/mol | Joback Method |
| hvap | 45.19 | kJ/mol | Joback Method |
| log10ws | -1.87 | | Crippen Method |
| logp | 1.781 | | Crippen Method |
| mcvol | 140.710 | ml/mol | McGowan Method |
| pc | 2989.32 | kPa | Joback Method |
| rinpol | 1485.00 | | NIST Webbook |
| rinpol | 1485.00 | | NIST Webbook |
| tb | 561.38 | K | Joback Method |
| tc | 794.80 | K | Joback Method |
| tf | 374.14 | K | Joback Method |
| vc | 0.536 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 384.96 | J/mol×K | 561.38 | Joback Method |
| cpg | 404.36 | J/mol×K | 600.28 | Joback Method |
| cpg | 422.47 | J/mol×K | 639.19 | Joback Method |
| cpg | 439.44 | J/mol×K | 678.09 | Joback Method |
| cpg | 455.46 | J/mol×K | 716.99 | Joback Method |
| cpg | 470.71 | J/mol×K | 755.90 | Joback Method |
| cpg | 485.34 | J/mol×K | 794.80 | 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=R44405&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |