# 1-((1S,3aR,4S,7R,7aR)-3a,7a-Dimethyloctahydro-1

**Inchi:** InChI=1S/C14H22O/c1-9(15)12-6-7-13(2)10-4-5-11(8-10)14(12,13)3/h10-12H,4-8H2,1-3
**InchiKey:** ZVJYJEILWCYOQE-UHFFFAOYSA-N
**Formula:** C14H22O
**SMILES:** CC(=O)C1CCC2(C)C3CCC(C3)C12C
**Mol. weight [g/mol]:** 206.32
**CAS:** 66748-84-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 81.83 | kJ/mol | Joback Method |
| hf | -242.83 | kJ/mol | Joback Method |
| hfus | 15.47 | kJ/mol | Joback Method |
| hvap | 50.50 | kJ/mol | Joback Method |
| log10ws | -3.44 | | Crippen Method |
| logp | 3.428 | | Crippen Method |
| mcvol | 177.110 | ml/mol | McGowan Method |
| pc | 2356.49 | kPa | Joback Method |
| rinpol | 1589.40 | | NIST Webbook |
| tb | 589.22 | K | Joback Method |
| tc | 815.60 | K | Joback Method |
| tf | 387.09 | K | Joback Method |
| vc | 0.682 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 497.75 | J/mol×K | 589.22 | Joback Method |
| cpg | 518.74 | J/mol×K | 626.95 | Joback Method |
| cpg | 538.31 | J/mol×K | 664.68 | Joback Method |
| cpg | 556.79 | J/mol×K | 702.41 | Joback Method |
| cpg | 574.48 | J/mol×K | 740.14 | Joback Method |
| cpg | 591.69 | J/mol×K | 777.87 | Joback Method |
| cpg | 608.72 | J/mol×K | 815.60 | 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=C66748843&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |