# 3-ethyl-5,7-dimethyl-1-adamantanol

**Inchi:** InChI=1S/C14H24O/c1-4-13-6-11(2)5-12(3,7-13)9-14(15,8-11)10-13/h15H,4-10H2,1-3H3
**InchiKey:** DYHYRNOUWAAUDI-UHFFFAOYSA-N
**Formula:** C14H24O
**SMILES:** CCC12CC3(C)CC(C)(CC(O)(C3)C1)C2
**Mol. weight [g/mol]:** 208.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 70.66 | kJ/mol | Joback Method |
| hf | -231.66 | kJ/mol | Joback Method |
| hfus | 4.29 | kJ/mol | Joback Method |
| hvap | 58.44 | kJ/mol | Joback Method |
| log10ws | -4.02 | | Crippen Method |
| logp | 3.508 | | Crippen Method |
| mcvol | 181.410 | ml/mol | McGowan Method |
| pc | 2746.90 | kPa | Joback Method |
| rinpol | 1421.00 | | NIST Webbook |
| rinpol | 1421.00 | | NIST Webbook |
| rinpol | 1440.00 | | NIST Webbook |
| rinpol | 1466.00 | | NIST Webbook |
| rinpol | 1454.00 | | NIST Webbook |
| ripol | 1909.00 | | NIST Webbook |
| ripol | 1948.00 | | NIST Webbook |
| ripol | 1932.00 | | NIST Webbook |
| ripol | 1909.00 | | NIST Webbook |
| tb | 632.68 | K | Joback Method |
| tc | 850.73 | K | Joback Method |
| tf | 450.02 | K | Joback Method |
| vc | 0.693 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 533.79 | J/mol×K | 632.68 | Joback Method |

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|---|---|---|---|---|
| cpg | 551.29 | J/mol×K | 669.02 | Joback Method |
| cpg | 568.13 | J/mol×K | 705.36 | Joback Method |
| cpg | 584.76 | J/mol×K | 741.71 | Joback Method |
| cpg | 601.64 | J/mol×K | 778.05 | Joback Method |
| cpg | 619.24 | J/mol×K | 814.39 | Joback Method |
| cpg | 638.01 | J/mol×K | 850.73 | Joback Method |

# 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=R304719&Units=SI |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |