# 2-Methyladamantane

**Other names:** Tricyclo[3.3.1.1
**Inchi:** InChI=1S/C11H18/c1-7-10-3-8-2-9(5-10)6-11(7)4-8/h7-11H,2-6H2,1H3
**InchiKey:** VMODAALDMAYACB-UHFFFAOYSA-N
**Formula:** C11H18
**SMILES:** CC1C2CC3CC(C2)CC1C3
**Mol. weight [g/mol]:** 150.26
**CAS:** 700-56-1

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -6684.40 ± 1.20 | kJ/mol | NIST Webbook |
| chs | -6676.00 ± 2.00 | kJ/mol | NIST Webbook |
| gf | 196.47 | kJ/mol | Joback Method |
| hf | -151.40 ± 4.00 | kJ/mol | NIST Webbook |
| hf | -152.00 ± 4.40 | kJ/mol | NIST Webbook |
| hfs | -216.70 ± 1.20 | kJ/mol | NIST Webbook |
| hfs | -225.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfus | 18.69 | kJ/mol | Joback Method |
| hsub | 73.60 | kJ/mol | NIST Webbook |
| hsub | 68.20 ± 1.30 | kJ/mol | NIST Webbook |
| hsub | 67.53 | kJ/mol | NIST Webbook |
| hsub | 68.00 ± 1.00 | kJ/mol | NIST Webbook |
| hsub | 64.70 | kJ/mol | NIST Webbook |
| hvap | 39.37 | kJ/mol | Joback Method |
| ie | 9.24 | eV | NIST Webbook |
| log10ws | -2.90 | | Crippen Method |
| logp | 3.079 | | Crippen Method |
| mcvol | 133.270 | ml/mol | McGowan Method |
| pc | 2698.60 | kPa | Joback Method |
| rinpol | 1175.00 | | NIST Webbook |
| rinpol | 1168.00 | | NIST Webbook |
| rinpol | 1175.00 | | NIST Webbook |
| rinpol | 1176.20 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| rinpol | 1175.00 | | NIST Webbook |
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1187.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1200.00 | | NIST Webbook |
| rinpol | 1162.00 | | NIST Webbook |
| rinpol | 1168.00 | | NIST Webbook |
| rinpol | 1175.00 | | NIST Webbook |
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| rinpol | 1196.00 | | NIST Webbook |
| rinpol | 1209.00 | | NIST Webbook |
| rinpol | 1168.00 | | NIST Webbook |
| rinpol | 1196.00 | | NIST Webbook |
| rinpol | 1196.00 | | NIST Webbook |
| rinpol | 1200.00 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| rinpol | 1166.00 | | NIST Webbook |
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1200.00 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| ripol | 1407.00 | | NIST Webbook |
| ripol | 1442.00 | | NIST Webbook |
| ripol | 1420.00 | | NIST Webbook |
| ripol | 1400.00 | | NIST Webbook |
| tb | 466.23 | K | Joback Method |
| tc | 676.61 | K | Joback Method |
| tf | 414.00 ± 0.50 | K | NIST Webbook |
| vc | 0.512 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 431.62 | J/mol×K | 676.61 | Joback Method |
| cpg | 415.85 | J/mol×K | 641.54 | Joback Method |
| cpg | 398.99 | J/mol×K | 606.48 | Joback Method |
| cpg | 380.97 | J/mol×K | 571.42 | Joback Method |
| cpg | 361.70 | J/mol×K | 536.36 | Joback Method |
| cpg | 341.08 | J/mol×K | 501.29 | Joback Method |
| cpg | 319.04 | J/mol×K | 466.23 | Joback Method |
| dvisc | 0.0005341 | Pa×s | 255.55 | Joback Method |
| dvisc | 0.0012554 | Pa×s | 466.23 | Joback Method |
| dvisc | 0.0011538 | Pa×s | 431.12 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0010446 | Pa×s | 396.00 | Joback Method |
| dvisc | 0.0009276 | Pa×s | 360.89 | Joback Method |
| dvisc | 0.0008029 | Pa×s | 325.78 | Joback Method |
| dvisc | 0.0006712 | Pa×s | 290.66 | Joback Method |
| hsubt | 67.50 ± 2.10 | kJ/mol | 320.00 | NIST Webbook |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C700561&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |

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