# 1-bromomethyladamantane

**Inchi:** InChI=1S/C11H17Br/c12-7-11-4-8-1-9(5-11)3-10(2-8)6-11/h8-10H,1-7H2
**InchiKey:** RLRBYCAVZBQANU-UHFFFAOYSA-N
**Formula:** C11H17Br
**SMILES:** BrCC12CC3CC(CC(C3)C1)C2
**Mol. weight [g/mol]:** 229.16

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 213.01 | kJ/mol | Joback Method |
| hf | -36.90 | kJ/mol | Joback Method |
| hfus | 16.61 | kJ/mol | Joback Method |
| hvap | 44.97 | kJ/mol | Joback Method |
| log10ws | -3.58 | | Crippen Method |
| logp | 3.598 | | Crippen Method |
| mcvol | 150.770 | ml/mol | McGowan Method |
| pc | 3163.27 | kPa | Joback Method |
| rinpol | 1508.00 | | NIST Webbook |
| rinpol | 1488.00 | | NIST Webbook |
| rinpol | 1526.00 | | NIST Webbook |
| rinpol | 1494.00 | | NIST Webbook |
| rinpol | 1494.00 | | NIST Webbook |
| rinpol | 1543.00 | | NIST Webbook |
| rinpol | 1543.00 | | NIST Webbook |
| rinpol | 1494.00 | | NIST Webbook |
| ripol | 1916.00 | | NIST Webbook |
| ripol | 1971.00 | | NIST Webbook |
| ripol | 1941.00 | | NIST Webbook |
| ripol | 1925.00 | | NIST Webbook |
| ripol | 1925.00 | | NIST Webbook |
| ripol | 1925.00 | | NIST Webbook |
| tb | 537.30 | K | Joback Method |
| tc | 773.48 | K | Joback Method |
| tf | 343.49 | K | Joback Method |
| vc | 0.574 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.61 | J/mol×K | 537.30 | Joback Method |
| cpg | 391.45 | J/mol×K | 576.66 | Joback Method |
| cpg | 409.61 | J/mol×K | 616.03 | Joback Method |
| cpg | 426.35 | J/mol×K | 655.39 | Joback Method |
| cpg | 441.92 | J/mol×K | 694.75 | Joback Method |
| cpg | 456.58 | J/mol×K | 734.11 | Joback Method |
| cpg | 470.57 | J/mol×K | 773.48 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R237699&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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