# Tricyclo[3.3.1.1(3,7)-]decane, 1-bromo-3,5-dimethyl-

**Other names:** 1-Bromo-3,5-dimethyladamantane
3,5-dimethyl-1-bromoadamantane
1-bromo-3,5-dimethyltricyclo[3.3.1.13,7]decane

**Inchi:** InChI=1S/C12H19Br/c1-10-3-9-4-11(2,6-10)8-12(13,5-9)7-10/h9H,3-8H2,1-2H3

**InchiKey:** QUCXLVDIVQWYJR-UHFFFAOYSA-N

**Formula:** C12H19Br

**SMILES:** CC12CC3CC(C)(C1)CC(Br)(C3)C2

**Mol. weight [g/mol]:** 243.18

**CAS:** 941-37-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 210.45 | kJ/mol | Joback Method |
| hf | -27.06 | kJ/mol | Joback Method |
| hfus | 6.60 | kJ/mol | Joback Method |
| hvap | 44.89 | kJ/mol | Joback Method |
| log10ws | -4.35 | | Crippen Method |
| logp | 4.130 | | Crippen Method |
| mcvol | 164.860 | ml/mol | McGowan Method |
| pc | 3142.03 | kPa | Joback Method |
| rinpol | 1417.00 | | NIST Webbook |
| rinpol | 1432.00 | | NIST Webbook |
| rinpol | 1448.00 | | NIST Webbook |
| rinpol | 1401.00 | | NIST Webbook |
| ripol | 1788.00 | | NIST Webbook |
| ripol | 1815.00 | | NIST Webbook |
| ripol | 1762.00 | | NIST Webbook |
| ripol | 1762.00 | | NIST Webbook |
| tb | 560.66 | K | Joback Method |
| tc | 812.64 | K | Joback Method |
| tf | 402.56 | K | Joback Method |
| vc | 0.625 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 418.51 | J/mol×K | 560.66 | Joback Method |
| cpg | 438.26 | J/mol×K | 602.66 | Joback Method |
| cpg | 456.22 | J/mol×K | 644.65 | Joback Method |
| cpg | 472.96 | J/mol×K | 686.65 | Joback Method |
| cpg | 489.07 | J/mol×K | 728.64 | Joback Method |
| cpg | 505.13 | J/mol×K | 770.64 | Joback Method |
| cpg | 521.70 | J/mol×K | 812.64 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C941377&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