# 5-Bromovaleric acid, 1-adamantylmethyl ester

**Inchi:** InChI=1S/C16H25BrO2/c17-4-2-1-3-15(18)19-11-16-8-12-5-13(9-16)7-14(6-12)10-16/h12
**InchiKey:** LDMGZPZQMNUSFN-UHFFFAOYSA-N
**Formula:** C16H25BrO2
**SMILES:** O=C(CCCCBr)OCC12CC3CC(CC(C3)C1)C2
**Mol. weight [g/mol]:** 329.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 21.19 | kJ/mol | Joback Method |
| hf | -384.90 | kJ/mol | Joback Method |
| hfus | 32.35 | kJ/mol | Joback Method |
| hvap | 65.25 | kJ/mol | Joback Method |
| log10ws | -4.53 | | Crippen Method |
| logp | 4.311 | | Crippen Method |
| mcvol | 228.660 | ml/mol | McGowan Method |
| pc | 2043.76 | kPa | Joback Method |
| rinpol | 2212.00 | | NIST Webbook |
| rinpol | 2212.00 | | NIST Webbook |
| tb | 727.99 | K | Joback Method |
| tc | 946.92 | K | Joback Method |
| tf | 472.00 | K | Joback Method |
| vc | 0.877 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 684.97 | J/mol×K | 727.99 | Joback Method |
| cpg | 704.03 | J/mol×K | 764.48 | Joback Method |
| cpg | 722.28 | J/mol×K | 800.97 | Joback Method |
| cpg | 739.92 | J/mol×K | 837.45 | Joback Method |
| cpg | 757.15 | J/mol×K | 873.94 | Joback Method |
| cpg | 774.18 | J/mol×K | 910.43 | Joback Method |
| cpg | 791.20 | J/mol×K | 946.92 | Joback Method |

# Sources

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|---|---|
| **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=U299982&Units=SI |

# Legend

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