# 6-Bromohexanoic acid, 4-methoxyphenyl ester

**Inchi:** InChI=1S/C13H17BrO3/c1-16-11-6-8-12(9-7-11)17-13(15)5-3-2-4-10-14/h6-9H,2-5,10H2
**InchiKey:** JSVXNJVKIMSPGN-UHFFFAOYSA-N
**Formula:** C13H17BrO3
**SMILES:** COc1ccc(OC(=O)CCCCCBr)cc1
**Mol. weight [g/mol]:** 301.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -163.24 | kJ/mol | Joback Method |
| hf | -437.28 | kJ/mol | Joback Method |
| hfus | 32.34 | kJ/mol | Joback Method |
| hvap | 65.47 | kJ/mol | Joback Method |
| log10ws | -4.01 | | Crippen Method |
| logp | 3.556 | | Crippen Method |
| mcvol | 201.080 | ml/mol | McGowan Method |
| pc | 2374.90 | kPa | Joback Method |
| rinpol | 2066.00 | | NIST Webbook |
| tb | 693.37 | K | Joback Method |
| tc | 906.36 | K | Joback Method |
| tf | 429.40 | K | Joback Method |
| vc | 0.759 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 510.37 | J/mol×K | 693.37 | Joback Method |
| cpg | 524.37 | J/mol×K | 728.87 | Joback Method |
| cpg | 537.49 | J/mol×K | 764.37 | Joback Method |
| cpg | 549.75 | J/mol×K | 799.87 | Joback Method |
| cpg | 561.17 | J/mol×K | 835.36 | Joback Method |
| cpg | 571.76 | J/mol×K | 870.86 | Joback Method |
| cpg | 581.53 | J/mol×K | 906.36 | Joback Method |
| dvisc | 0.0008983 | Pa×s | 429.40 | Joback Method |
| dvisc | 0.0005470 | Pa×s | 473.40 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003624 | Pa×s | 517.39 | Joback Method |
| dvisc | 0.0002561 | Pa×s | 561.38 | Joback Method |
| dvisc | 0.0001904 | Pa×s | 605.38 | Joback Method |
| dvisc | 0.0001473 | Pa×s | 649.38 | Joback Method |
| dvisc | 0.0001178 | Pa×s | 693.37 | Joback Method |

# Sources

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|---|---|
| **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=U307616&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |