# Pentanamide, N-(4-bromophenyl)-5-chloro-

**Inchi:** InChI=1S/C11H13BrClNO/c12-9-4-6-10(7-5-9)14-11(15)3-1-2-8-13/h4-7H,1-3,8H2,(H,14,
**InchiKey:** CFOVGBMBEDOVGW-UHFFFAOYSA-N
**Formula:** C11H13BrClNO
**SMILES:** O=C(CCCCCl)Nc1ccc(Br)cc1
**Mol. weight [g/mol]:** 290.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.38 | kJ/mol | Joback Method |
| hf | -93.83 | kJ/mol | Joback Method |
| hfus | 34.08 | kJ/mol | Joback Method |
| hvap | 67.02 | kJ/mol | Joback Method |
| log10ws | -4.25 | | Crippen Method |
| logp | 3.797 | | Crippen Method |
| mcvol | 183.380 | ml/mol | McGowan Method |
| pc | 2921.84 | kPa | Joback Method |
| rinpol | 2210.00 | | NIST Webbook |
| tb | 690.37 | K | Joback Method |
| tc | 917.82 | K | Joback Method |
| tf | 444.98 | K | Joback Method |
| vc | 0.696 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 432.83 | J/mol×K | 690.37 | Joback Method |
| cpg | 444.79 | J/mol×K | 728.28 | Joback Method |
| cpg | 455.89 | J/mol×K | 766.19 | Joback Method |
| cpg | 466.18 | J/mol×K | 804.09 | Joback Method |
| cpg | 475.72 | J/mol×K | 842.00 | Joback Method |
| cpg | 484.55 | J/mol×K | 879.91 | Joback Method |
| cpg | 492.73 | J/mol×K | 917.82 | Joback Method |

# Sources

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|---|---|
| **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=U307362&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |