# Benzamide, 2-bromo-N-(2-bromobenzoyl)-N-propyl-

**Inchi:** InChI=1S/C17H15Br2NO2/c1-2-11-20(16(21)12-7-3-5-9-14(12)18)17(22)13-8-4-6-10-15(

**InchiKey:** YBOHFNJJBGOLEY-UHFFFAOYSA-N

**Formula:** C17H15Br2NO2

**SMILES:** CCCN(C(=O)c1ccccc1Br)C(=O)c1ccccc1Br

**Mol. weight [g/mol]:** 425.12

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 179.40 | kJ/mol | Joback Method |
| hf | -49.06 | kJ/mol | Joback Method |
| hfus | 43.88 | kJ/mol | Joback Method |
| hvap | 87.72 | kJ/mol | Joback Method |
| log10ws | -6.75 | | Crippen Method |
| logp | 4.904 | | Crippen Method |
| mcvol | 250.990 | ml/mol | McGowan Method |
| pc | 2613.74 | kPa | Joback Method |
| rinpol | 2621.00 | | NIST Webbook |
| rinpol | 2621.00 | | NIST Webbook |
| tb | 904.18 | K | Joback Method |
| tc | 1157.20 | K | Joback Method |
| tf | 611.16 | K | Joback Method |
| vc | 0.925 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 663.15 | J/mol×K | 904.18 | Joback Method |
| cpg | 674.41 | J/mol×K | 946.35 | Joback Method |
| cpg | 684.77 | J/mol×K | 988.52 | Joback Method |
| cpg | 694.36 | J/mol×K | 1030.69 | Joback Method |
| cpg | 703.30 | J/mol×K | 1072.86 | Joback Method |
| cpg | 711.72 | J/mol×K | 1115.03 | Joback Method |
| cpg | 719.74 | J/mol×K | 1157.20 | Joback Method |

# Sources

| | |
|---|---|
| **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=U407066&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |