# Benzamide, 2-bromo-N-(2-bromobenzoyl)-N-(3-methylbutyl)-

**Inchi:** InChI=1S/C19H19Br2NO2/c1-13(2)11-12-22(18(23)14-7-3-5-9-16(14)20)19(24)15-8-4-6-

**InchiKey:** CHZOVBDEBYJQCV-UHFFFAOYSA-N

**Formula:** C19H19Br2NO2

**SMILES:** CC(C)CCN(C(=O)c1ccccc1Br)C(=O)c1ccccc1Br

**Mol. weight [g/mol]:** 453.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 193.80 | kJ/mol | Joback Method |
| hf | -95.62 | kJ/mol | Joback Method |
| hfus | 45.54 | kJ/mol | Joback Method |
| hvap | 91.78 | kJ/mol | Joback Method |
| log10ws | -7.34 | | Crippen Method |
| logp | 5.540 | | Crippen Method |
| mcvol | 279.170 | ml/mol | McGowan Method |
| pc | 2183.60 | kPa | Joback Method |
| rinpol | 2753.00 | | NIST Webbook |
| rinpol | 2753.00 | | NIST Webbook |
| tb | 949.50 | K | Joback Method |
| tc | 1199.01 | K | Joback Method |
| tf | 618.70 | K | Joback Method |
| vc | 1.032 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 776.71 | J/mol×K | 949.50 | Joback Method |
| cpg | 788.72 | J/mol×K | 991.08 | Joback Method |
| cpg | 799.83 | J/mol×K | 1032.67 | Joback Method |
| cpg | 810.19 | J/mol×K | 1074.25 | Joback Method |
| cpg | 819.91 | J/mol×K | 1115.84 | Joback Method |
| cpg | 829.13 | J/mol×K | 1157.42 | Joback Method |
| cpg | 837.98 | J/mol×K | 1199.01 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407069&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 |

# 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 |