# Benzamide, 3-methoxy-N-(3-methoxybenzoyl)-N-methyl-

**Inchi:** InChI=1S/C17H17NO4/c1-18(16(19)12-6-4-8-14(10-12)21-2)17(20)13-7-5-9-15(11-13)22

**InchiKey:** SQQGHUZPDMSBNL-UHFFFAOYSA-N

**Formula:** C17H17NO4

**SMILES:** COc1cccc(C(=O)N(C)C(=O)c2cccc(OC)c2)c1

**Mol. weight [g/mol]:** 299.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -59.24 | kJ/mol | Joback Method |
| hf | -366.16 | kJ/mol | Joback Method |
| hfus | 35.68 | kJ/mol | Joback Method |
| hvap | 79.67 | kJ/mol | Joback Method |
| log10ws | -3.82 | | Crippen Method |
| logp | 2.616 | | Crippen Method |
| mcvol | 227.730 | ml/mol | McGowan Method |
| pc | 2208.29 | kPa | Joback Method |
| rinpol | 2380.00 | | NIST Webbook |
| rinpol | 2380.00 | | NIST Webbook |
| tb | 816.70 | K | Joback Method |
| tc | 1046.56 | K | Joback Method |
| tf | 536.02 | K | Joback Method |
| vc | 0.838 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 651.87 | J/mol×K | 816.70 | Joback Method |
| cpg | 665.52 | J/mol×K | 855.01 | Joback Method |
| cpg | 677.94 | J/mol×K | 893.32 | Joback Method |
| cpg | 689.16 | J/mol×K | 931.63 | Joback Method |
| cpg | 699.22 | J/mol×K | 969.94 | Joback Method |
| cpg | 708.14 | J/mol×K | 1008.25 | Joback Method |
| cpg | 715.96 | J/mol×K | 1046.56 | 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=U407521&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 |