# 1-Benzyl-3-(3-methoxybenzyl)urea

**Inchi:** InChI=1S/C16H18N2O2/c1-20-15-9-5-8-14(10-15)12-18-16(19)17-11-13-6-3-2-4-7-13/h2
**InchiKey:** ZSKPRGWARSZXBG-UHFFFAOYSA-N
**Formula:** C16H18N2O2
**SMILES:** COc1cccc(CNC(=O)NCc2ccccc2)c1
**Mol. weight [g/mol]:** 270.33
**CAS:** 1007825-60-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 243.89 | kJ/mol | Joback Method |
| hf | -49.84 | kJ/mol | Joback Method |
| hfus | 37.87 | kJ/mol | Joback Method |
| hvap | 78.45 | kJ/mol | Joback Method |
| log10ws | -4.55 | | Crippen Method |
| logp | 2.695 | | Crippen Method |
| mcvol | 216.180 | ml/mol | McGowan Method |
| pc | 2414.74 | kPa | Joback Method |
| rinpol | 2630.00 | | NIST Webbook |
| rinpol | 2630.00 | | NIST Webbook |
| tb | 800.45 | K | Joback Method |
| tc | 1030.49 | K | Joback Method |
| tf | 512.92 | K | Joback Method |
| vc | 0.809 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 624.75 | J/mol×K | 800.45 | Joback Method |
| cpg | 638.87 | J/mol×K | 838.79 | Joback Method |
| cpg | 651.81 | J/mol×K | 877.13 | Joback Method |
| cpg | 663.63 | J/mol×K | 915.47 | Joback Method |
| cpg | 674.38 | J/mol×K | 953.81 | Joback Method |
| cpg | 684.12 | J/mol×K | 992.15 | Joback Method |
| cpg | 692.90 | J/mol×K | 1030.49 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1007825606&Units=SI |

# 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 |

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