

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	ZSKPRGWARSZXBG-UHFFFAOYSA-N
<b>Formula:</b>	C16H18N2O2
<b>SMILES:</b>	COc1cccc(CNC(=O)NCc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	270.33
<b>CAS:</b>	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
mvol	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/molxK	800.45	Joback Method
cpg	638.87	J/molxK	838.79	Joback Method
cpg	651.81	J/molxK	877.13	Joback Method
cpg	663.63	J/molxK	915.47	Joback Method
cpg	674.38	J/molxK	953.81	Joback Method
cpg	684.12	J/molxK	992.15	Joback Method
cpg	692.90	J/molxK	1030.49	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1007825606&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1007825606&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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