

# 1-Benzyl-3-(5-carbomethoxyamyl) urea

<b>Inchi:</b>	InChI=1S/C15H22N2O3/c1-20-14(18)10-6-3-7-11-16-15(19)17-12-13-8-4-2-5-9-13/h2,4-5
<b>InchiKey:</b>	LVPSBDGKJIEFEL-UHFFFAOYSA-N
<b>Formula:</b>	C15H22N2O3
<b>SMILES:</b>	COC(=O)CCCCCNC(=O)NCc1ccccc1
<b>Mol. weight [g/mol]:</b>	278.35
<b>CAS:</b>	92700-37-3

## Physical Properties

Property code	Value	Unit	Source
gf	3.77	kJ/mol	Joback Method
hf	-366.84	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	80.03	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.219		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
tb	799.78	K	Joback Method
tc	1006.10	K	Joback Method
tf	512.64	K	Joback Method
vc	0.868	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.49	J/molxK	799.78	Joback Method
cpg	691.37	J/molxK	834.17	Joback Method
cpg	704.26	J/molxK	868.55	Joback Method
cpg	716.19	J/molxK	902.94	Joback Method
cpg	727.19	J/molxK	937.33	Joback Method
cpg	737.31	J/molxK	971.71	Joback Method
cpg	746.57	J/molxK	1006.10	Joback Method

# Sources

<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=C92700373&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92700373&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvap:</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>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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