

Benzamide, N-tetrahydrofurfuryl-3-methyl-

Inchi:	InChI=1S/C13H17NO2/c1-10-4-2-5-11(8-10)13(15)14-9-12-6-3-7-16-12/h2,4-5,8,12H,3,6
InchiKey:	JZSLUHRDIFJWGK-UHFFFAOYSA-N
Formula:	C13H17NO2
SMILES:	<chem>Cc1cccc(C(=O)NCC2CCCO2)c1</chem>
Mol. weight [g/mol]:	219.28

Physical Properties

Property code	Value	Unit	Source
gf	72.26	kJ/mol	Joback Method
hf	-217.22	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	1.904		Crippen Method
mvol	176.830	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	674.77	K	Joback Method
tc	906.14	K	Joback Method
tf	415.27	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.40	J/molxK	674.77	Joback Method
cpg	507.14	J/molxK	713.33	Joback Method
cpg	522.66	J/molxK	751.89	Joback Method
cpg	537.01	J/molxK	790.46	Joback Method
cpg	550.25	J/molxK	829.02	Joback Method
cpg	562.44	J/molxK	867.58	Joback Method
cpg	573.65	J/molxK	906.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U307111&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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