

Benzamide, N-tetrahydrofurfuryl-3-methoxy-

Inchi:	InChI=1S/C13H17NO3/c1-16-11-5-2-4-10(8-11)13(15)14-9-12-6-3-7-17-12/h2,4-5,8,12H,
InchiKey:	CXNMRTSCFAKPIT-UHFFFAOYSA-N
Formula:	C13H17NO3
SMILES:	<chem>COc1cccc(C(=O)NCC2CCCO2)c1</chem>
Mol. weight [g/mol]:	235.28

Physical Properties

Property code	Value	Unit	Source
gf	-32.74	kJ/mol	Joback Method
hf	-349.44	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.604		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinqol	2084.00		NIST Webbook
tb	697.19	K	Joback Method
tc	925.39	K	Joback Method
tf	437.50	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.11	J/molxK	697.19	Joback Method
cpg	533.36	J/molxK	735.22	Joback Method
cpg	548.41	J/molxK	773.26	Joback Method
cpg	562.32	J/molxK	811.29	Joback Method
cpg	575.12	J/molxK	849.32	Joback Method
cpg	586.84	J/molxK	887.35	Joback Method
cpg	597.53	J/molxK	925.39	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=U306966&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
mccvol:	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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