Benzamide, N-tetrahydrofurfuryl-2-methoxy-

Inchi: InChI=1S/C13H17NO3/c1-16-12-7-3-2-6-11(12)13(15)14-9-10-5-4-8-17-10/h2-3,6-7,10H
InchiKey: UVKDWTOQXFIEJZ-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: COc1ccccc1C(=O)NCC1CCCO1
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
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	697.19	K	Joback Method
tc	925.39	K	Joback Method
tf	437.50	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.11	J/mol×K	697.19	Joback Method
cpg	533.36	J/mol×K	735.22	Joback Method
cpg	548.41	J/mol×K	773.26	Joback Method
cpg	562.32	J/mol×K	811.29	Joback Method
cpg	575.12	J/mol×K	849.32	Joback Method
cpg	586.84	J/mol×K	887.35	Joback Method
cpg	597.53	J/mol×K	925.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307056&Units=SI
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

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