Benzamide, N-tetrahydrofurfuryl-2-methyl-

Inchi: InChI=1S/C13H17NO2/c1-10-5-2-3-7-12(10)13(15)14-9-11-6-4-8-16-11/h2-3,5,7,11H,4,6
InchiKey: NRSKFBXGJXDGQD-UHFFFAOYSA-N
Formula: C13H17NO2
SMILES: Cc1ccccc1C(=O)NCC1CCCO1
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
mcvol	176.830	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	674.77	K	Joback Method
tc	906.14	K	Joback Method
tf	415.27	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=U307001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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