Benzamide, N-tetrahydrofurfuryl-2-fluoro-

Inchi: InChI=1S/C12H14FNO2/c13-11-6-2-1-5-10(11)12(15)14-8-9-4-3-7-16-9/h1-2,5-6,9H,3-4,
InchiKey: DTKPNMGQXXHNPW-UHFFFAOYSA-N
Formula: C12H14FNO2
SMILES: O=C(NCC1CCCO1)c1ccccc1F
Mol. weight [g/mol]: 223.24

Physical Properties

Property code	Value	Unit	Source
gf	-130.97	kJ/mol	Joback Method
hf	-392.69	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	62.38	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.734		Crippen Method
mcvol	164.510	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	651.16	K	Joback Method
tc	876.35	K	Joback Method
tf	404.59	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.69	J/mol×K	651.16	Joback Method
cpg	462.24	J/mol×K	688.69	Joback Method
cpg	476.66	J/mol×K	726.22	Joback Method
cpg	490.00	J/mol×K	763.75	Joback Method
cpg	502.31	J/mol×K	801.28	Joback Method
cpg	513.66	J/mol×K	838.82	Joback Method
cpg	524.09	J/mol×K	876.35	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=U307078&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