

Benzamide, N-tetrahydrofurfuryl-3-fluoro-

Inchi:	InChI=1S/C12H14FNO2/c13-10-4-1-3-9(7-10)12(15)14-8-11-5-2-6-16-11/h1,3-4,7,11H,2
InchiKey:	LAYIKHUZIUKLPK-UHFFFAOYSA-N
Formula:	C12H14FNO2
SMILES:	O=C(NCC1CCCO1)c1cccc(F)c1
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
mvol	164.510	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	651.16	K	Joback Method
tc	876.35	K	Joback Method
tf	404.59	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.69	J/molxK	651.16	Joback Method
cpg	462.24	J/molxK	688.69	Joback Method
cpg	476.66	J/molxK	726.22	Joback Method
cpg	490.00	J/molxK	763.75	Joback Method
cpg	502.31	J/molxK	801.28	Joback Method
cpg	513.66	J/molxK	838.82	Joback Method
cpg	524.09	J/molxK	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=U307162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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