

Benzamide, N-tetrahydrofurfuryl-2,6-difluoro-

Inchi: InChI=1S/C12H13F2NO2/c13-9-4-1-5-10(14)11(9)12(16)15-7-8-3-2-6-17-8/h1,4-5,8H,2-3
InchiKey: GZOWKIITIDVBIP-UHFFFAOYSA-N
Formula: C12H13F2NO2
SMILES: O=C(NCC1CCCO1)c1c(F)cccc1F
Mol. weight [g/mol]: 241.23

Physical Properties

Property code	Value	Unit	Source
gf	-335.41	kJ/mol	Joback Method
hf	-600.27	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	62.22	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	1.874		Crippen Method
mcvol	166.280	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	655.41	K	Joback Method
tc	871.46	K	Joback Method
tf	417.70	K	Joback Method
vc	0.638	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.96	J/mol×K	655.41	Joback Method
cpg	468.56	J/mol×K	691.42	Joback Method
cpg	482.16	J/mol×K	727.43	Joback Method
cpg	494.79	J/mol×K	763.43	Joback Method
cpg	506.49	J/mol×K	799.44	Joback Method
cpg	517.31	J/mol×K	835.45	Joback Method
cpg	527.29	J/mol×K	871.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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