

Benzamide, 3,4-difluoro-N-propyl-

Inchi:	InChI=1S/C10H11F2NO/c1-2-5-13-10(14)7-3-4-8(11)9(12)6-7/h3-4,6H,2,5H2,1H3,(H,13,
InchiKey:	NLOAFYAOJJJSMQ-UHFFFAOYSA-N
Formula:	C10H11F2NO
SMILES:	CCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	199.20

Physical Properties

Property code	Value	Unit	Source
gf	-302.68	kJ/mol	Joback Method
hf	-487.47	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	53.00	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.105		Crippen Method
mcvol	143.090	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpola	1535.00		NIST Webbook
rinpola	1535.00		NIST Webbook
tb	567.42	K	Joback Method
tc	764.66	K	Joback Method
tf	357.69	K	Joback Method
vc	0.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.50	J/mol×K	567.42	Joback Method
cpg	351.52	J/mol×K	600.29	Joback Method
cpg	362.88	J/mol×K	633.17	Joback Method
cpg	373.59	J/mol×K	666.04	Joback Method
cpg	383.68	J/mol×K	698.91	Joback Method
cpg	393.16	J/mol×K	731.78	Joback Method
cpg	402.07	J/mol×K	764.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407788&Units=SI

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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