Benzamide, 2,5-difluoro-N-propyl-

Inchi: InChI=1S/C10H11F2NO/c1-2-5-13-10(14)8-6-7(11)3-4-9(8)12/h3-4,6H,2,5H2,1H3,(H,13,
InchiKey: OCXMIBPSRURZIR-UHFFFAOYSA-N
Formula: C10H11F2NO
SMILES: CCCNC(=O)c1cc(F)ccc1F
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
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
tb	567.42	K	Joback Method
tc	764.66	K	Joback Method
tf	357.69	K	Joback Method
vc	0.565	m3/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:	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=U407582&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