Benzamide, 2,6-difluoro-3-methyl-N-propyl-

Inchi: InChI=1S/C11H13F2NO/c1-3-6-14-11(15)9-8(12)5-4-7(2)10(9)13/h4-5H,3,6H2,1-2H3,(H,
InchiKey: DMVDMUCWOGAZTI-UHFFFAOYSA-N
Formula: C11H13F2NO
SMILES: CCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 213.22

Physical Properties

Property code	Value	Unit	Source
gf	-303.89	kJ/mol	Joback Method
hf	-519.58	kJ/mol	Joback Method
hfus	29.98	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	2.413		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	595.28	K	Joback Method
tc	790.86	K	Joback Method
tf	381.48	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.00	J/mol×K	595.28	Joback Method
cpg	398.55	J/mol×K	627.88	Joback Method
cpg	410.44	J/mol×K	660.47	Joback Method
cpg	421.68	J/mol×K	693.07	Joback Method
cpg	432.30	J/mol×K	725.67	Joback Method
cpg	442.31	J/mol×K	758.27	Joback Method
cpg	451.72	J/mol×K	790.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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