Benzamide, 3-chloro-2-fluoro-N-propyl-

Inchi: InChI=1S/C10H11ClFNO/c1-2-6-13-10(14)7-4-3-5-8(11)9(7)12/h3-5H,2,6H2,1H3,(H,13,1
InchiKey: KAIHCBUCZFZZCK-UHFFFAOYSA-N
Formula: C10H11ClFNO
SMILES: CCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 215.65

Physical Properties

Property code	Value	Unit	Source
gf	-119.80	kJ/mol	Joback Method
hf	-307.10	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	58.20	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.619		Crippen Method
mcvol	153.560	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	605.58	K	Joback Method
tc	816.44	K	Joback Method
tf	387.02	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.45	J/mol×K	605.58	Joback Method
cpg	368.24	J/mol×K	640.72	Joback Method
cpg	379.31	J/mol×K	675.87	Joback Method
cpg	389.68	J/mol×K	711.01	Joback Method
cpg	399.38	J/mol×K	746.15	Joback Method
cpg	408.44	J/mol×K	781.30	Joback Method
cpg	416.87	J/mol×K	816.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407819&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
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