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

Inchi: InChI=1S/C13H17ClFNO/c1-2-3-4-5-9-16-13(17)10-7-6-8-11(14)12(10)15/h6-8H,2-5,9H2
InchiKey: GXRPDIYYIRZGBX-UHFFFAOYSA-N
Formula: C13H17ClFNO
SMILES: CCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 257.73

Physical Properties

Property code	Value	Unit	Source
gf	-94.54	kJ/mol	Joback Method
hf	-369.02	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.789		Crippen Method
mcvol	195.830	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	674.22	K	Joback Method
tc	876.08	K	Joback Method
tf	420.83	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.99	J/mol×K	674.22	Joback Method
cpg	518.68	J/mol×K	707.86	Joback Method
cpg	531.56	J/mol×K	741.51	Joback Method
cpg	543.66	J/mol×K	775.15	Joback Method
cpg	555.00	J/mol×K	808.79	Joback Method
cpg	565.62	J/mol×K	842.44	Joback Method
cpg	575.54	J/mol×K	876.08	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=U407824&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