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

Inchi: InChI=1S/C15H21ClFNO/c1-2-3-4-5-6-7-11-18-15(19)12-9-8-10-13(16)14(12)17/h8-10H,
InchiKey: UGGKOLYDYUUVPO-UHFFFAOYSA-N
Formula: C15H21ClFNO
SMILES: CCCCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 285.79

Physical Properties

Property code	Value	Unit	Source
gf	-77.70	kJ/mol	Joback Method
hf	-410.30	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.569		Crippen Method
mcvol	224.010	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	719.98	K	Joback Method
tc	917.66	K	Joback Method
tf	443.37	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.87	J/mol×K	719.98	Joback Method
cpg	625.47	J/mol×K	752.93	Joback Method
cpg	639.20	J/mol×K	785.87	Joback Method
cpg	652.11	J/mol×K	818.82	Joback Method
cpg	664.23	J/mol×K	851.76	Joback Method
cpg	675.58	J/mol×K	884.71	Joback Method
cpg	686.21	J/mol×K	917.66	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=U407827&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