3-Chloro-2-fluorobenzamide, N-(2-octyl)-

Inchi: InChI=1S/C15H21ClFNO/c1-3-4-5-6-8-11(2)18-15(19)12-9-7-10-13(16)14(12)17/h7,9-11
InchiKey: BBPNKNMZAYDYKS-UHFFFAOYSA-N
Formula: C15H21ClFNO
SMILES: CCCCCCC(C)NC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 285.79

Physical Properties

Property code	Value	Unit	Source
gf	-80.14	kJ/mol	Joback Method
hf	-415.58	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.568		Crippen Method
mcvol	224.010	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2059.00		NIST Webbook
tb	719.54	K	Joback Method
tc	920.23	K	Joback Method
tf	428.37	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.41	J/mol×K	719.54	Joback Method
cpg	626.24	J/mol×K	752.99	Joback Method
cpg	640.18	J/mol×K	786.44	Joback Method
cpg	653.26	J/mol×K	819.89	Joback Method
cpg	665.51	J/mol×K	853.33	Joback Method
cpg	676.97	J/mol×K	886.78	Joback Method
cpg	687.68	J/mol×K	920.23	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=U358132&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