3-Chloro-2-fluorobenzamide, N,N-dihexyl-

Inchi: InChI=1S/C19H29ClFNO/c1-3-5-7-9-14-22(15-10-8-6-4-2)19(23)16-12-11-13-17(20)18(1
InchiKey: XSNYXOGPWYXVNN-UHFFFAOYSA-N
Formula: C19H29ClFNO
SMILES: CCCCCCN(CCCCCC)C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 341.89

Physical Properties

Property code	Value	Unit	Source
gf	-22.63	kJ/mol	Joback Method
hf	-478.80	kJ/mol	Joback Method
hfus	50.13	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.082		Crippen Method
mcvol	280.370	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	2389.00		NIST Webbook
tb	773.77	K	Joback Method
tc	964.69	K	Joback Method
tf	468.26	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.01	J/mol×K	773.77	Joback Method
cpg	834.67	J/mol×K	805.59	Joback Method
cpg	850.38	J/mol×K	837.41	Joback Method
cpg	865.17	J/mol×K	869.23	Joback Method
cpg	879.09	J/mol×K	901.05	Joback Method
cpg	892.20	J/mol×K	932.87	Joback Method
cpg	904.52	J/mol×K	964.69	Joback Method

Sources

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=U358135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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