3-Chloro-2-fluorobenzamide, N-pentyl-

Inchi: InChI=1S/C12H15ClFNO/c1-2-3-4-8-15-12(16)9-6-5-7-10(13)11(9)14/h5-7H,2-4,8H2,1H3
InchiKey: LFMPIITXVHOGLI-UHFFFAOYSA-N
Formula: C12H15ClFNO
SMILES: CCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 243.71

Physical Properties

Property code	Value	Unit	Source
gf	-102.96	kJ/mol	Joback Method
hf	-348.38	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	62.66	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.399		Crippen Method
mcvol	181.740	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1906.00		NIST Webbook
tb	651.34	K	Joback Method
tc	855.88	K	Joback Method
tf	409.56	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.02	J/mol×K	651.34	Joback Method
cpg	467.16	J/mol×K	685.43	Joback Method
cpg	479.52	J/mol×K	719.52	Joback Method
cpg	491.12	J/mol×K	753.61	Joback Method
cpg	501.99	J/mol×K	787.70	Joback Method
cpg	512.16	J/mol×K	821.79	Joback Method
cpg	521.65	J/mol×K	855.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358131&Units=SI
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

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