3-Chloro-2-fluorobenzoic acid, 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C13H6ClF2NO4/c14-9-3-1-2-8(12(9)16)13(18)21-11-6-7(15)4-5-10(11)17(19)2

InchiKey: HUKPKYZHEGUWMG-UHFFFAOYSA-N

Formula: C13H6ClF2NO4

SMILES: O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1cccc(Cl)c1F

Mol. weight [g/mol]: 313.64

Physical Properties

Property code	Value	Unit	Source
gf	-355.04	kJ/mol	Joback Method
hf	-547.99	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	80.23	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	3.746		Crippen Method
mcvol	187.150	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	2185.00		NIST Webbook
tb	834.22	K	Joback Method
tc	1083.37	K	Joback Method
tf	586.06	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.83	J/mol×K	834.22	Joback Method
cpg	495.85	J/mol×K	875.75	Joback Method
cpg	503.87	J/mol×K	917.27	Joback Method
cpg	510.91	J/mol×K	958.80	Joback Method
cpg	517.00	J/mol×K	1000.32	Joback Method
cpg	522.18	J/mol×K	1041.85	Joback Method
cpg	526.46	J/mol×K	1083.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357731&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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