3-Chlorobenzoic acid, 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C13H7ClFNO4/c14-9-3-1-2-8(6-9)13(17)20-12-7-10(15)4-5-11(12)16(18)19/h1

InchiKey: SSRSDIPPPNHLEQ-UHFFFAOYSA-N

Formula: C13H7ClFNO4

SMILES: O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1cccc(Cl)c1

Mol. weight [g/mol]: 295.65

Physical Properties

Property code	Value	Unit	Source
gf	-150.60	kJ/mol	Joback Method
hf	-340.41	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	3.607		Crippen Method
mcvol	185.380	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	829.97	K	Joback Method
tc	1088.79	K	Joback Method
tf	572.95	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.19	J/mol×K	829.97	Joback Method
cpg	490.81	J/mol×K	873.11	Joback Method
cpg	499.34	J/mol×K	916.24	Joback Method
cpg	506.81	J/mol×K	959.38	Joback Method
cpg	513.28	J/mol×K	1002.52	Joback Method
cpg	518.79	J/mol×K	1045.66	Joback Method
cpg	523.38	J/mol×K	1088.79	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=U357788&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

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