

3-Chloro-2-fluorobenzoic acid, 4-nitrophenyl ester

Inchi:	InChI=1S/C13H7ClFNO4/c14-11-3-1-2-10(12(11)15)13(17)20-9-6-4-8(5-7-9)16(18)19/h1
InchiKey:	LEJYFBCFPBXCFZ-UHFFFAOYSA-N
Formula:	C13H7ClFNO4
SMILES:	O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccc(Cl)c1F
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
mvol	185.380	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	829.97	K	Joback Method
tc	1088.79	K	Joback Method
tf	572.95	K	Joback Method
vc	0.721	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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