

3-Chloro-2-fluorobenzoic acid, 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C13H6Cl3FO2/c14-8-4-2-6-10(11(8)16)19-13(18)7-3-1-5-9(15)12(7)17/h1-6H
InchiKey:	YPRNASYQICTJQC-UHFFFAOYSA-N
Formula:	C13H6Cl3FO2
SMILES:	O=C(Oc1cccc(Cl)c1Cl)c1cccc(Cl)c1F
Mol. weight [g/mol]:	319.54

Physical Properties

Property code	Value	Unit	Source
gf	-219.64	kJ/mol	Joback Method
hf	-372.60	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.005		Crippen Method
mcvol	192.440	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	757.97	K	Joback Method
tc	1004.92	K	Joback Method
tf	501.70	K	Joback Method
vc	0.737	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.57	J/molxK	757.97	Joback Method
cpg	445.33	J/molxK	799.13	Joback Method
cpg	454.17	J/molxK	840.29	Joback Method
cpg	462.11	J/molxK	881.45	Joback Method
cpg	469.18	J/molxK	922.61	Joback Method
cpg	475.40	J/molxK	963.76	Joback Method
cpg	480.80	J/molxK	1004.92	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=U357334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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