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

Inchi: InChI=1S/C9H5Cl4FO2/c10-6-3-1-2-5(7(6)14)8(15)16-4-9(11,12)13/h1-3H,4H2
InchiKey: AEOVZPHQDDCQEM-UHFFFAOYSA-N
Formula: C9H5Cl4FO2
SMILES: O=C(OCC(Cl)(Cl)Cl)c1cccc(Cl)c1F
Mol. weight [g/mol]: 305.94

Physical Properties

Property code	Value	Unit	Source
gf	-355.56	kJ/mol	Joback Method
hf	-528.12	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	63.81	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.006		Crippen Method
mcvol	172.080	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	664.01	K	Joback Method
tc	900.27	K	Joback Method
tf	437.50	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.87	J/mol×K	664.01	Joback Method
cpg	365.41	J/mol×K	703.39	Joback Method
cpg	373.18	J/mol×K	742.76	Joback Method
cpg	380.22	J/mol×K	782.14	Joback Method
cpg	386.59	J/mol×K	821.52	Joback Method
cpg	392.33	J/mol×K	860.90	Joback Method
cpg	397.48	J/mol×K	900.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360583&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