3-Fluorobenzoic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C9H6Cl3FO2/c10-9(11,12)5-15-8(14)6-2-1-3-7(13)4-6/h1-4H,5H2
InchiKey: SCVBNVMGLBENQO-UHFFFAOYSA-N
Formula: C9H6Cl3FO2
SMILES: O=C(OCC(Cl)(Cl)Cl)c1cccc(F)c1
Mol. weight [g/mol]: 271.50

Physical Properties

Property code	Value	Unit	Source
gf	-334.00	kJ/mol	Joback Method
hf	-500.91	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	58.76	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.353		Crippen Method
mcvol	159.840	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	621.60	K	Joback Method
tc	853.91	K	Joback Method
tf	395.06	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.14	J/mol×K	621.60	Joback Method
cpg	347.88	J/mol×K	660.32	Joback Method
cpg	356.79	J/mol×K	699.04	Joback Method
cpg	364.92	J/mol×K	737.76	Joback Method
cpg	372.31	J/mol×K	776.48	Joback Method
cpg	379.00	J/mol×K	815.19	Joback Method
cpg	385.06	J/mol×K	853.91	Joback Method

Sources

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=U355664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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