3-Fluoro-4-trifluoromethylbenzoic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H5Cl3F4O2/c11-9(12,13)4-19-8(18)5-1-2-6(7(14)3-5)10(15,16)17/h1-3H,4H

InchiKey: QEDVZDHKDKWUNB-UHFFFAOYSA-N

Formula: C10H5Cl3F4O2

SMILES: O=C(OCC(Cl)(Cl)Cl)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 339.50

Physical Properties

Property code	Value	Unit	Source
gf	-916.80	kJ/mol	Joback Method
hf	-1130.10	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.372		Crippen Method
mcvol	179.240	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1527.00		NIST Webbook
tb	644.04	K	Joback Method
tc	854.96	K	Joback Method
tf	423.04	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.56	J/mol×K	644.04	Joback Method
cpg	420.71	J/mol×K	679.19	Joback Method
cpg	429.07	J/mol×K	714.35	Joback Method
cpg	436.68	J/mol×K	749.50	Joback Method
cpg	443.59	J/mol×K	784.65	Joback Method
cpg	449.88	J/mol×K	819.80	Joback Method
cpg	455.58	J/mol×K	854.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360596&Units=SI

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