Succinic acid, 1,1,1-trifluoroprop-2-yl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C9H10Cl3F3O4/c1-5(9(13,14)15)19-7(17)3-2-6(16)18-4-8(10,11)12/h5H,2-4H2

InchiKey: NWSWYNHQKIDTDF-UHFFFAOYSA-N

Formula: C9H10Cl3F3O4

SMILES: CC(OC(=O)CCC(=O)OCC(Cl)(Cl)Cl)C(F)(F)F

Mol. weight [g/mol]: 345.53

Physical Properties

Property code	Value	Unit	Source
gf	-1059.92	kJ/mol	Joback Method
hf	-1377.02	kJ/mol	Joback Method
hfus	28.12	kJ/mol	Joback Method
hvap	61.66	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.174		Crippen Method
mcvol	194.580	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
tb	661.10	K	Joback Method
tc	854.41	K	Joback Method
tf	416.88	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.90	J/mol×K	661.10	Joback Method
cpg	485.71	J/mol×K	693.32	Joback Method
cpg	494.82	J/mol×K	725.54	Joback Method
cpg	503.25	J/mol×K	757.76	Joback Method
cpg	511.04	J/mol×K	789.97	Joback Method
cpg	518.22	J/mol×K	822.19	Joback Method
cpg	524.81	J/mol×K	854.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390226&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