Succinic acid, 2,2-dichloroethyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C9H9Cl2F5O4/c10-5(11)3-19-6(17)1-2-7(18)20-4-8(12,13)9(14,15)16/h5H,1-4H

InchiKey: WTONREYSDGKWQD-UHFFFAOYSA-N

Formula: C9H9Cl2F5O4

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

Mol. weight [g/mol]: 347.06

Physical Properties

Property code	Value	Unit	Source
gf	-1437.61	kJ/mol	Joback Method
hf	-1753.50	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.854		Crippen Method
mcvol	185.880	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
tb	622.21	K	Joback Method
tc	797.37	K	Joback Method
tf	388.14	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.52	J/mol×K	622.21	Joback Method
cpg	478.37	J/mol×K	651.40	Joback Method
cpg	487.58	J/mol×K	680.60	Joback Method
cpg	496.20	J/mol×K	709.79	Joback Method
cpg	504.23	J/mol×K	738.99	Joback Method
cpg	511.70	J/mol×K	768.18	Joback Method
cpg	518.64	J/mol×K	797.37	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=U390864&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