Succinic acid, 2,2,3,3-tetrafluoropropyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C9H9Cl3F4O4/c10-9(11,12)4-20-6(18)2-1-5(17)19-3-8(15,16)7(13)14/h7H,1-4H

InchiKey: FVJAVKKTVABPCH-UHFFFAOYSA-N

Formula: C9H9Cl3F4O4

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

Mol. weight [g/mol]: 363.52

Physical Properties

Property code	Value	Unit	Source
gf	-1254.73	kJ/mol	Joback Method
hf	-1573.13	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.124		Crippen Method
mcvol	196.350	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
tb	660.37	K	Joback Method
tc	846.52	K	Joback Method
tf	417.47	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.00	J/mol×K	660.37	Joback Method
cpg	493.39	J/mol×K	691.40	Joback Method
cpg	502.12	J/mol×K	722.42	Joback Method
cpg	510.22	J/mol×K	753.45	Joback Method
cpg	517.70	J/mol×K	784.47	Joback Method
cpg	524.60	J/mol×K	815.50	Joback Method
cpg	530.96	J/mol×K	846.52	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=U390227&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