Succinic acid, 2,2-dichloroethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C12H9Cl2F3O4/c13-8(14)5-20-9(18)3-4-10(19)21-7-2-1-6(15)11(16)12(7)17/h1

InchiKey: JHCRWTPPMWTGNJ-UHFFFAOYSA-N

Formula: C12H9Cl2F3O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)OCC(Cl)Cl

Mol. weight [g/mol]: 345.10

Physical Properties

Property code	Value	Unit	Source
gf	-944.89	kJ/mol	Joback Method
hf	-1203.58	kJ/mol	Joback Method
hfus	39.39	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.136		Crippen Method
mcvol	200.850	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1967.00		NIST Webbook
tb	740.39	K	Joback Method
tc	940.47	K	Joback Method
tf	479.91	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.94	J/mol×K	740.39	Joback Method
cpg	515.83	J/mol×K	773.74	Joback Method
cpg	525.01	J/mol×K	807.08	Joback Method
cpg	533.48	J/mol×K	840.43	Joback Method
cpg	541.24	J/mol×K	873.78	Joback Method
cpg	548.28	J/mol×K	907.12	Joback Method
cpg	554.60	J/mol×K	940.47	Joback Method

Sources

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=U390759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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