Succinic acid, 1,1,1-trifluoroprop-2-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C13H10F6O4/c1-6(13(17,18)19)22-9(20)4-5-10(21)23-8-3-2-7(14)11(15)12(8)1

InchiKey: CYPFGRWRNLUEAQ-UHFFFAOYSA-N

Formula: C13H10F6O4

SMILES: CC(OC(=O)CCC(=O)Oc1ccc(F)c(F)c1F)C(F)(F)F

Mol. weight [g/mol]: 344.21

Physical Properties

Property code	Value	Unit	Source
gf	-1494.20	kJ/mol	Joback Method
hf	-1789.82	kJ/mol	Joback Method
hfus	35.42	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.283		Crippen Method
mcvol	195.770	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	682.99	K	Joback Method
tc	862.43	K	Joback Method
tf	435.53	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.96	J/mol×K	682.99	Joback Method
cpg	548.02	J/mol×K	712.90	Joback Method
cpg	558.42	J/mol×K	742.80	Joback Method
cpg	568.15	J/mol×K	772.71	Joback Method
cpg	577.24	J/mol×K	802.62	Joback Method
cpg	585.69	J/mol×K	832.52	Joback Method
cpg	593.52	J/mol×K	862.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390753&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