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

Inchi: InChI=1S/C17H25F3O4/c1-12(2)6-5-7-13(3)10-11-23-15(21)8-9-16(22)24-14(4)17(18,19

InchiKey: XSNRVDTXUWIVPF-JLHYYAGUSA-N

Formula: C17H25F3O4

SMILES: CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 350.37

Physical Properties

Property code	Value	Unit	Source
gf	-816.27	kJ/mol	Joback Method
hf	-1271.31	kJ/mol	Joback Method
hfus	41.45	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.497		Crippen Method
mcvol	261.980	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	743.16	K	Joback Method
tc	925.18	K	Joback Method
tf	376.78	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.16	J/mol×K	743.16	Joback Method
cpg	783.35	J/mol×K	773.50	Joback Method
cpg	797.69	J/mol×K	803.83	Joback Method
cpg	811.23	J/mol×K	834.17	Joback Method
cpg	824.01	J/mol×K	864.51	Joback Method
cpg	836.07	J/mol×K	894.85	Joback Method
cpg	847.46	J/mol×K	925.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391207&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