Succinic acid, 1,1,1-trifluoroprop-2-yl 10-chlorodecyl ester

Inchi: InChI=1S/C17H28ClF3O4/c1-14(17(19,20)21)25-16(23)11-10-15(22)24-13-9-7-5-3-2-4-6

InchiKey: JTAHBZHOLRMGJG-UHFFFAOYSA-N

Formula: C17H28ClF3O4

SMILES: CC(OC(=O)CCC(=O)OCCCCCCCCCCCCl)C(F)(F)F

Mol. weight [g/mol]: 388.85

Physical Properties

Property code	Value	Unit	Source
gf	-971.54	kJ/mol	Joback Method
hf	-1501.91	kJ/mol	Joback Method
hfus	47.86	kJ/mol	Joback Method
hvap	72.00	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.163		Crippen Method
mcvol	282.820	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2148.00		NIST Webbook
tb	772.51	K	Joback Method
tc	950.70	K	Joback Method
tf	444.78	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.34	J/mol×K	772.51	Joback Method
cpg	862.59	J/mol×K	802.21	Joback Method
cpg	876.96	J/mol×K	831.91	Joback Method
cpg	890.48	J/mol×K	861.61	Joback Method
cpg	903.16	J/mol×K	891.30	Joback Method
cpg	915.04	J/mol×K	921.00	Joback Method
cpg	926.14	J/mol×K	950.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390401&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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