Succinic acid, 1,1,1-trifluoroprop-2-yl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C14H20ClF3O4/c1-9(14(16,17)18)22-13(20)7-6-12(19)21-8-10-4-2-3-5-11(10)1

InchiKey: IYZXMVMCVSTQII-UHFFFAOYSA-N

Formula: C14H20ClF3O4

SMILES: CC(OC(=O)CCC(=O)OCC1CCCCC1Cl)C(F)(F)F

Mol. weight [g/mol]: 344.75

Physical Properties

Property code	Value	Unit	Source
gf	-980.06	kJ/mol	Joback Method
hf	-1406.01	kJ/mol	Joback Method
hfus	33.00	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.601		Crippen Method
mcvol	229.690	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1878.00		NIST Webbook
rinpol	1878.00		NIST Webbook
tb	718.75	K	Joback Method
tc	912.54	K	Joback Method
tf	414.11	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.26	J/mol×K	718.75	Joback Method
cpg	691.18	J/mol×K	751.05	Joback Method
cpg	706.04	J/mol×K	783.35	Joback Method
cpg	719.86	J/mol×K	815.65	Joback Method
cpg	732.66	J/mol×K	847.95	Joback Method
cpg	744.46	J/mol×K	880.24	Joback Method
cpg	755.28	J/mol×K	912.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391396&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