Succinic acid, 1,1,1-trifluoroprop-2-yl 3-chlorophenyl ester

Inchi: InChI=1S/C13H12ClF3O4/c1-8(13(15,16)17)20-11(18)5-6-12(19)21-10-4-2-3-9(14)7-10/h

InchiKey: PDKNAXJOWNBFCK-UHFFFAOYSA-N

Formula: C13H12ClF3O4

SMILES: CC(OC(=O)CCC(=O)Oc1cccc(Cl)c1)C(F)(F)F

Mol. weight [g/mol]: 324.68

Physical Properties

Property code	Value	Unit	Source
gf	-902.44	kJ/mol	Joback Method
hf	-1194.29	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.520		Crippen Method
mcvol	202.700	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	712.65	K	Joback Method
tc	914.04	K	Joback Method
tf	438.64	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.11	J/mol×K	712.65	Joback Method
cpg	551.87	J/mol×K	746.21	Joback Method
cpg	562.77	J/mol×K	779.78	Joback Method
cpg	572.84	J/mol×K	813.34	Joback Method
cpg	582.12	J/mol×K	846.91	Joback Method
cpg	590.62	J/mol×K	880.47	Joback Method
cpg	598.36	J/mol×K	914.04	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=U389845&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