Succinic acid, 3-chlorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C14H11ClF6O4/c15-8-2-1-3-9(6-8)25-11(23)5-4-10(22)24-7-13(17,18)12(16)14

InchiKey: FVYYZPUSRCHDOB-UHFFFAOYSA-N

Formula: C14H11ClF6O4

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

Mol. weight [g/mol]: 392.68

Physical Properties

Property code	Value	Unit	Source
gf	-1475.61	kJ/mol	Joback Method
hf	-1812.01	kJ/mol	Joback Method
hfus	35.57	kJ/mol	Joback Method
hvap	64.51	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.105		Crippen Method
mcvol	222.100	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	730.11	K	Joback Method
tc	918.46	K	Joback Method
tf	454.10	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.61	J/mol×K	730.11	Joback Method
cpg	629.63	J/mol×K	761.50	Joback Method
cpg	639.82	J/mol×K	792.89	Joback Method
cpg	649.23	J/mol×K	824.28	Joback Method
cpg	657.89	J/mol×K	855.67	Joback Method
cpg	665.85	J/mol×K	887.07	Joback Method
cpg	673.14	J/mol×K	918.46	Joback Method

Sources

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=U390808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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