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

Inchi: InChI=1S/C14H10Cl2F6O4/c15-7-2-1-3-8(11(7)16)26-10(24)5-4-9(23)25-6-13(18,19)12(1

InchiKey: FWPCWKXYQINLLY-UHFFFAOYSA-N

Formula: C14H10Cl2F6O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 427.12

Physical Properties

Property code	Value	Unit	Source
gf	-1497.17	kJ/mol	Joback Method
hf	-1839.22	kJ/mol	Joback Method
hfus	39.38	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.758		Crippen Method
mcvol	234.340	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	772.52	K	Joback Method
tc	966.17	K	Joback Method
tf	496.54	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.28	J/mol×K	772.52	Joback Method
cpg	650.18	J/mol×K	804.80	Joback Method
cpg	659.28	J/mol×K	837.07	Joback Method
cpg	667.62	J/mol×K	869.35	Joback Method
cpg	675.24	J/mol×K	901.62	Joback Method
cpg	682.19	J/mol×K	933.90	Joback Method
cpg	688.50	J/mol×K	966.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390811&Units=SI

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