Succinic acid, 2,4,6-trichlorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C14H9Cl3F6O4/c15-6-3-7(16)11(8(17)4-6)27-10(25)2-1-9(24)26-5-13(19,20)12

InchiKey: WADJFOLLLYRODJ-UHFFFAOYSA-N

Formula: C14H9Cl3F6O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 461.57

Physical Properties

Property code	Value	Unit	Source
gf	-1518.73	kJ/mol	Joback Method
hf	-1866.43	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	74.61	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.411		Crippen Method
mcvol	246.580	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
tb	814.93	K	Joback Method
tc	1014.04	K	Joback Method
tf	538.98	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.73	J/mol×K	814.93	Joback Method
cpg	668.56	J/mol×K	848.11	Joback Method
cpg	676.61	J/mol×K	881.30	Joback Method
cpg	683.93	J/mol×K	914.48	Joback Method
cpg	690.56	J/mol×K	947.67	Joback Method
cpg	696.54	J/mol×K	980.85	Joback Method
cpg	701.90	J/mol×K	1014.04	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=U390813&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