Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C15H9Cl3F8O4/c16-6-3-8(18)9(4-7(6)17)30-11(28)2-1-10(27)29-5-13(21,22)15

InchiKey: GXYOVYQZMGSFIU-UHFFFAOYSA-N

Formula: C15H9Cl3F8O4

SMILES: O=C(CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 511.58

Physical Properties

Property code	Value	Unit	Source
gf	-1897.09	kJ/mol	Joback Method
hf	-2288.04	kJ/mol	Joback Method
hfus	44.52	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.047		Crippen Method
mcvol	264.210	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	833.12	K	Joback Method
tc	1029.25	K	Joback Method
tf	553.85	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.25	J/mol×K	833.12	Joback Method
cpg	738.85	J/mol×K	865.81	Joback Method
cpg	746.71	J/mol×K	898.50	Joback Method
cpg	753.86	J/mol×K	931.18	Joback Method
cpg	760.38	J/mol×K	963.87	Joback Method
cpg	766.31	J/mol×K	996.56	Joback Method
cpg	771.72	J/mol×K	1029.25	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=U389960&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