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

Inchi: InChI=1S/C15H7Cl5F8O4/c16-6-7(17)9(19)11(10(20)8(6)18)32-5(30)2-1-4(29)31-3-13(23

InchiKey: YSKVIVKLNSYSJT-UHFFFAOYSA-N

Formula: C15H7Cl5F8O4

SMILES: O=C(CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 580.47

Physical Properties

Property code	Value	Unit	Source
gf	-1940.21	kJ/mol	Joback Method
hf	-2342.46	kJ/mol	Joback Method
hfus	52.14	kJ/mol	Joback Method
hvap	83.99	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.353		Crippen Method
mcvol	288.690	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	917.94	K	Joback Method
tc	1127.64	K	Joback Method
tf	638.73	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.67	J/mol×K	917.94	Joback Method
cpg	769.38	J/mol×K	952.89	Joback Method
cpg	775.41	J/mol×K	987.84	Joback Method
cpg	780.83	J/mol×K	1022.79	Joback Method
cpg	785.68	J/mol×K	1057.74	Joback Method
cpg	790.05	J/mol×K	1092.69	Joback Method
cpg	793.99	J/mol×K	1127.64	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=U390045&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