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

Inchi: InChI=1S/C15H7F13O4/c16-6-7(17)9(19)11(10(20)8(6)18)32-5(30)2-1-4(29)31-3-13(23,2

InchiKey: VPFGJWOJVVKHGG-UHFFFAOYSA-N

Formula: C15H7F13O4

SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 498.19

Physical Properties

Property code	Value	Unit	Source
gf	-2854.61	kJ/mol	Joback Method
hf	-3244.31	kJ/mol	Joback Method
hfus	46.55	kJ/mol	Joback Method
hvap	57.98	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.782		Crippen Method
mcvol	236.340	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	1582.00		NIST Webbook
tb	727.14	K	Joback Method
tc	892.91	K	Joback Method
tf	492.08	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.51	J/mol×K	727.14	Joback Method
cpg	709.45	J/mol×K	754.77	Joback Method
cpg	718.71	J/mol×K	782.40	Joback Method
cpg	727.33	J/mol×K	810.03	Joback Method
cpg	735.32	J/mol×K	837.66	Joback Method
cpg	742.73	J/mol×K	865.28	Joback Method
cpg	749.58	J/mol×K	892.91	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=U390346&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