Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 1-phenylpropyl ester

Inchi: InChI=1S/C18H18F8O4/c1-2-12(11-6-4-3-5-7-11)30-14(28)9-8-13(27)29-10-16(21,22)18

InchiKey: LSXXJSZBNZCDOL-UHFFFAOYSA-N

Formula: C18H18F8O4

SMILES: CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccccc1

Mol. weight [g/mol]: 450.32

Physical Properties

Property code	Value	Unit	Source
gf	-1809.59	kJ/mol	Joback Method
hf	-2273.61	kJ/mol	Joback Method
hfus	37.34	kJ/mol	Joback Method
hvap	65.05	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.175		Crippen Method
mcvol	269.760	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	1878.00		NIST Webbook
rinpol	1878.00		NIST Webbook
tb	774.09	K	Joback Method
tc	956.40	K	Joback Method
tf	445.34	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.11	J/mol×K	774.09	Joback Method
cpg	842.20	J/mol×K	804.48	Joback Method
cpg	854.35	J/mol×K	834.86	Joback Method
cpg	865.62	J/mol×K	865.25	Joback Method
cpg	876.07	J/mol×K	895.63	Joback Method
cpg	885.75	J/mol×K	926.02	Joback Method
cpg	894.74	J/mol×K	956.40	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=U389921&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