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

Inchi: InChI=1S/C21H16F8O4/c22-18(23)20(26,27)21(28,29)19(24,25)12-32-16(30)10-11-17(3

InchiKey: NVHWSQQUMUOYQA-UHFFFAOYSA-N

Formula: C21H16F8O4

SMILES: O=C(CCC(=O)Oc1ccc(-c2ccccc2)cc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 484.34

Physical Properties

Property code	Value	Unit	Source
gf	-1679.11	kJ/mol	Joback Method
hf	-2105.19	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	75.05	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	5.753		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	2547.00		NIST Webbook
rinpol	2547.00		NIST Webbook
tb	874.83	K	Joback Method
tc	1078.31	K	Joback Method
tf	533.09	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.04	J/mol×K	874.83	Joback Method
cpg	912.61	J/mol×K	908.74	Joback Method
cpg	923.21	J/mol×K	942.66	Joback Method
cpg	932.94	J/mol×K	976.57	Joback Method
cpg	941.88	J/mol×K	1010.48	Joback Method
cpg	950.13	J/mol×K	1044.39	Joback Method
cpg	957.78	J/mol×K	1078.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390080&Units=SI
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

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