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

Inchi: InChI=1S/C17H16F8O4/c1-9-4-3-5-11(10(9)2)29-13(27)7-6-12(26)28-8-15(20,21)17(24,2

InchiKey: PXKLQQZUZCPCFN-UHFFFAOYSA-N

Formula: C17H16F8O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1C

Mol. weight [g/mol]: 436.29

Physical Properties

Property code	Value	Unit	Source
gf	-1834.83	kJ/mol	Joback Method
hf	-2270.63	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.703		Crippen Method
mcvol	255.670	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	761.61	K	Joback Method
tc	942.89	K	Joback Method
tf	474.11	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.32	J/mol×K	761.61	Joback Method
cpg	783.75	J/mol×K	791.82	Joback Method
cpg	795.31	J/mol×K	822.04	Joback Method
cpg	806.04	J/mol×K	852.25	Joback Method
cpg	816.00	J/mol×K	882.46	Joback Method
cpg	825.24	J/mol×K	912.67	Joback Method
cpg	833.80	J/mol×K	942.89	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=U390014&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