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

Inchi: InChI=1S/C17H16F8O4/c18-14(19)16(22,23)17(24,25)15(20,21)10-29-13(27)7-6-12(26)2

InchiKey: BPOQOGPKAHOLMW-UHFFFAOYSA-N

Formula: C17H16F8O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCCc1ccccc1

Mol. weight [g/mol]: 436.29

Physical Properties

Property code	Value	Unit	Source
gf	-1815.57	kJ/mol	Joback Method
hf	-2247.69	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	63.21	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.267		Crippen Method
mcvol	255.670	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	751.65	K	Joback Method
tc	931.13	K	Joback Method
tf	449.07	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.24	J/mol×K	751.65	Joback Method
cpg	785.88	J/mol×K	781.56	Joback Method
cpg	797.62	J/mol×K	811.48	Joback Method
cpg	808.51	J/mol×K	841.39	Joback Method
cpg	818.61	J/mol×K	871.31	Joback Method
cpg	827.98	J/mol×K	901.22	Joback Method
cpg	836.67	J/mol×K	931.13	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=U389742&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