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

Inchi: InChI=1S/C17H14F8O5/c1-9(26)10-2-4-11(5-3-10)30-13(28)7-6-12(27)29-8-15(20,21)17

InchiKey: IBZMJZVJUKBKTE-UHFFFAOYSA-N

Formula: C17H14F8O5

SMILES: CC(=O)c1ccc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 450.28

Physical Properties

Property code	Value	Unit	Source
gf	-1954.12	kJ/mol	Joback Method
hf	-2371.74	kJ/mol	Joback Method
hfus	39.49	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.289		Crippen Method
mcvol	257.240	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	810.50	K	Joback Method
tc	999.61	K	Joback Method
tf	511.52	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.26	J/mol×K	810.50	Joback Method
cpg	797.26	J/mol×K	842.02	Joback Method
cpg	807.38	J/mol×K	873.54	Joback Method
cpg	816.68	J/mol×K	905.06	Joback Method
cpg	825.23	J/mol×K	936.57	Joback Method
cpg	833.08	J/mol×K	968.09	Joback Method
cpg	840.29	J/mol×K	999.61	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=U389908&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