Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C17H16F8O5/c1-9-3-4-10(28-2)11(7-9)30-13(27)6-5-12(26)29-8-15(20,21)17(2

InchiKey: KELUEXLJGVBASS-UHFFFAOYSA-N

Formula: C17H16F8O5

SMILES: COc1ccc(C)cc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 452.29

Physical Properties

Property code	Value	Unit	Source
gf	-1939.83	kJ/mol	Joback Method
hf	-2402.85	kJ/mol	Joback Method
hfus	38.69	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.403		Crippen Method
mcvol	261.540	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	784.03	K	Joback Method
tc	967.15	K	Joback Method
tf	496.34	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.40	J/mol×K	784.03	Joback Method
cpg	810.57	J/mol×K	814.55	Joback Method
cpg	821.85	J/mol×K	845.07	Joback Method
cpg	832.28	J/mol×K	875.59	Joback Method
cpg	841.89	J/mol×K	906.11	Joback Method
cpg	850.73	J/mol×K	936.63	Joback Method
cpg	858.85	J/mol×K	967.15	Joback Method

Sources

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=U390952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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