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

Inchi: InChI=1S/C17H22F8O4/c1-9-5-10(2)7-11(6-9)29-13(27)4-3-12(26)28-8-15(20,21)17(24,2

InchiKey: XLOMALSLXABOJX-UHFFFAOYSA-N

Formula: C17H22F8O4

SMILES: CC1CC(C)CC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)C1

Mol. weight [g/mol]: 442.34

Physical Properties

Property code	Value	Unit	Source
gf	-1918.95	kJ/mol	Joback Method
hf	-2470.58	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	60.75	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.849		Crippen Method
mcvol	268.570	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	735.18	K	Joback Method
tc	910.36	K	Joback Method
tf	421.55	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.13	J/mol×K	735.18	Joback Method
cpg	875.42	J/mol×K	764.38	Joback Method
cpg	890.64	J/mol×K	793.57	Joback Method
cpg	904.83	J/mol×K	822.77	Joback Method
cpg	918.04	J/mol×K	851.97	Joback Method
cpg	930.30	J/mol×K	881.16	Joback Method
cpg	941.66	J/mol×K	910.36	Joback Method

Sources

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=U391390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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