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

Inchi: InChI=1S/C15H20F8O4/c1-3-4-5-9(2)27-11(25)7-6-10(24)26-8-13(18,19)15(22,23)14(20

InchiKey: JALHNAQYBGSRRN-UHFFFAOYSA-N

Formula: C15H20F8O4

SMILES: CCCCC(C)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 416.30

Physical Properties

Property code	Value	Unit	Source
gf	-1947.26	kJ/mol	Joback Method
hf	-2448.22	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.603		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1228.56	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	678.77	K	Joback Method
tc	839.25	K	Joback Method
tf	385.11	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.43	J/mol×K	678.77	Joback Method
cpg	762.29	J/mol×K	705.52	Joback Method
cpg	775.37	J/mol×K	732.26	Joback Method
cpg	787.69	J/mol×K	759.01	Joback Method
cpg	799.29	J/mol×K	785.76	Joback Method
cpg	810.20	J/mol×K	812.51	Joback Method
cpg	820.46	J/mol×K	839.25	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=U390678&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