Succinic acid, dec-2-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C18H28F6O4/c1-3-4-5-6-7-8-9-13(2)28-15(26)11-10-14(25)27-12-17(20,21)16

InchiKey: KSLBXHGIMIODSH-UHFFFAOYSA-N

Formula: C18H28F6O4

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

Mol. weight [g/mol]: 422.40

Physical Properties

Property code	Value	Unit	Source
gf	-1535.22	kJ/mol	Joback Method
hf	-2109.17	kJ/mol	Joback Method
hfus	44.56	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.528		Crippen Method
mcvol	289.980	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1846.00		NIST Webbook
tb	752.10	K	Joback Method
tc	922.86	K	Joback Method
tf	415.32	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.38	J/mol×K	752.10	Joback Method
cpg	915.18	J/mol×K	780.56	Joback Method
cpg	930.08	J/mol×K	809.02	Joback Method
cpg	944.12	J/mol×K	837.48	Joback Method
cpg	957.33	J/mol×K	865.94	Joback Method
cpg	969.74	J/mol×K	894.40	Joback Method
cpg	981.40	J/mol×K	922.86	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=U390809&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