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

Inchi: InChI=1S/C13H18F6O4/c1-7(2)8(3)23-10(21)5-4-9(20)22-6-12(15,16)11(14)13(17,18)19/

InchiKey: YGNMDEASYJKIKU-UHFFFAOYSA-N

Formula: C13H18F6O4

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

Mol. weight [g/mol]: 352.27

Physical Properties

Property code	Value	Unit	Source
gf	-1579.76	kJ/mol	Joback Method
hf	-2011.25	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.433		Crippen Method
mcvol	219.530	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
tb	637.26	K	Joback Method
tc	800.71	K	Joback Method
tf	343.97	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.35	J/mol×K	637.26	Joback Method
cpg	636.98	J/mol×K	664.50	Joback Method
cpg	649.88	J/mol×K	691.74	Joback Method
cpg	662.07	J/mol×K	718.99	Joback Method
cpg	673.58	J/mol×K	746.23	Joback Method
cpg	684.42	J/mol×K	773.47	Joback Method
cpg	694.63	J/mol×K	800.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390800&Units=SI
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

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