Succinic acid, 3-methylbut-2-en-1-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C13H16F6O4/c1-8(2)5-6-22-9(20)3-4-10(21)23-7-12(15,16)11(14)13(17,18)19/

InchiKey: FDJSLBNCSKEXNM-UHFFFAOYSA-N

Formula: C13H16F6O4

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

Mol. weight [g/mol]: 350.25

Physical Properties

Property code	Value	Unit	Source
gf	-1503.21	kJ/mol	Joback Method
hf	-1893.26	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	55.00	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.355		Crippen Method
mcvol	215.230	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
tb	642.18	K	Joback Method
tc	807.90	K	Joback Method
tf	354.93	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.97	J/mol×K	642.18	Joback Method
cpg	613.78	J/mol×K	669.80	Joback Method
cpg	625.87	J/mol×K	697.42	Joback Method
cpg	637.28	J/mol×K	725.04	Joback Method
cpg	648.03	J/mol×K	752.66	Joback Method
cpg	658.15	J/mol×K	780.28	Joback Method
cpg	667.69	J/mol×K	807.90	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=U390802&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