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

Inchi: InChI=1S/C14H20F6O4/c1-4-9(8(2)3)24-11(22)6-5-10(21)23-7-13(16,17)12(15)14(18,19)

InchiKey: DZXFGGUIOPVCPJ-UHFFFAOYSA-N

Formula: C14H20F6O4

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

Mol. weight [g/mol]: 366.30

Physical Properties

Property code	Value	Unit	Source
gf	-1571.34	kJ/mol	Joback Method
hf	-2031.89	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	56.41	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.823		Crippen Method
mcvol	233.620	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	660.14	K	Joback Method
tc	824.16	K	Joback Method
tf	355.24	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.37	J/mol×K	660.14	Joback Method
cpg	690.47	J/mol×K	687.48	Joback Method
cpg	703.80	J/mol×K	714.81	Joback Method
cpg	716.40	J/mol×K	742.15	Joback Method
cpg	728.28	J/mol×K	769.49	Joback Method
cpg	739.48	J/mol×K	796.83	Joback Method
cpg	750.01	J/mol×K	824.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390801&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

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