Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C14H18F8O4/c1-7(2)8(3)26-10(24)5-4-9(23)25-6-12(17,18)14(21,22)13(19,20)

InchiKey: VJQGNQKVBWZVRR-UHFFFAOYSA-N

Formula: C14H18F8O4

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

Mol. weight [g/mol]: 402.28

Physical Properties

Property code	Value	Unit	Source
gf	-1958.12	kJ/mol	Joback Method
hf	-2432.86	kJ/mol	Joback Method
hfus	29.42	kJ/mol	Joback Method
hvap	53.48	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.068		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
tb	655.45	K	Joback Method
tc	815.85	K	Joback Method
tf	358.84	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.01	J/mol×K	655.45	Joback Method
cpg	708.59	J/mol×K	682.18	Joback Method
cpg	721.39	J/mol×K	708.92	Joback Method
cpg	733.44	J/mol×K	735.65	Joback Method
cpg	744.77	J/mol×K	762.38	Joback Method
cpg	755.42	J/mol×K	789.12	Joback Method
cpg	765.42	J/mol×K	815.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390579&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