Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C13H10F14O4/c14-7(12(23,24)25)9(17,18)3-30-5(28)1-2-6(29)31-4-10(19,20)

InchiKey: BKKYGOFBSMCUCD-UHFFFAOYSA-N

Formula: C13H10F14O4

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

Mol. weight [g/mol]: 496.19

Physical Properties

Property code	Value	Unit	Source
gf	-3127.28	kJ/mol	Joback Method
hf	-3601.10	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.560		Crippen Method
mcvol	233.690	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
tb	622.17	K	Joback Method
tc	767.08	K	Joback Method
tf	370.95	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.10	J/mol×K	622.17	Joback Method
cpg	707.74	J/mol×K	646.32	Joback Method
cpg	718.63	J/mol×K	670.47	Joback Method
cpg	728.81	J/mol×K	694.62	Joback Method
cpg	738.32	J/mol×K	718.78	Joback Method
cpg	747.20	J/mol×K	742.93	Joback Method
cpg	755.48	J/mol×K	767.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390799&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