Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl pent-4-en-2-yl ester

Inchi: InChI=1S/C14H16F8O4/c1-3-4-8(2)26-10(24)6-5-9(23)25-7-12(17,18)14(21,22)13(19,20)

InchiKey: JSGWQBREWPDYLP-UHFFFAOYSA-N

Formula: C14H16F8O4

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

Mol. weight [g/mol]: 400.26

Physical Properties

Property code	Value	Unit	Source
gf	-1867.84	kJ/mol	Joback Method
hf	-2302.15	kJ/mol	Joback Method
hfus	31.66	kJ/mol	Joback Method
hvap	53.20	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.989		Crippen Method
mcvol	232.860	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	652.57	K	Joback Method
tc	812.62	K	Joback Method
tf	372.08	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.84	J/mol×K	652.57	Joback Method
cpg	684.73	J/mol×K	679.24	Joback Method
cpg	696.85	J/mol×K	705.92	Joback Method
cpg	708.25	J/mol×K	732.59	Joback Method
cpg	718.96	J/mol×K	759.27	Joback Method
cpg	729.02	J/mol×K	785.94	Joback Method
cpg	738.45	J/mol×K	812.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391151&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