Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl but-3-en-1-yl ester

Inchi: InChI=1S/C13H14F8O4/c1-2-3-6-24-8(22)4-5-9(23)25-7-11(16,17)13(20,21)12(18,19)10(

InchiKey: DLORXODKWFNZPS-UHFFFAOYSA-N

Formula: C13H14F8O4

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

Mol. weight [g/mol]: 386.24

Physical Properties

Property code	Value	Unit	Source
gf	-1873.82	kJ/mol	Joback Method
hf	-2276.23	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.600		Crippen Method
mcvol	218.770	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	630.13	K	Joback Method
tc	787.47	K	Joback Method
tf	375.81	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.41	J/mol×K	630.13	Joback Method
cpg	631.66	J/mol×K	656.35	Joback Method
cpg	643.20	J/mol×K	682.58	Joback Method
cpg	654.06	J/mol×K	708.80	Joback Method
cpg	664.26	J/mol×K	735.03	Joback Method
cpg	673.85	J/mol×K	761.25	Joback Method
cpg	682.85	J/mol×K	787.47	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=U391185&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