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

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

InchiKey: VOWFNBNMEKSCIN-UHFFFAOYSA-N

Formula: C14H16F8O4

SMILES: C=C(C)CCOC(=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	-1873.95	kJ/mol	Joback Method
hf	-2306.66	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.990		Crippen Method
mcvol	232.860	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	652.89	K	Joback Method
tc	812.71	K	Joback Method
tf	373.12	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.10	J/mol×K	652.89	Joback Method
cpg	683.91	J/mol×K	679.53	Joback Method
cpg	695.97	J/mol×K	706.16	Joback Method
cpg	707.32	J/mol×K	732.80	Joback Method
cpg	717.99	J/mol×K	759.44	Joback Method
cpg	728.01	J/mol×K	786.07	Joback Method
cpg	737.43	J/mol×K	812.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391130&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