Succinic acid, 3-methylbut-2-en-1-yl 2,2,3,3,4,4,5,5-octafluoropentyl 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: FSANVZYARBVRGY-UHFFFAOYSA-N

Formula: C14H16F8O4

SMILES: CC(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	-1881.57	kJ/mol	Joback Method
hf	-2314.87	kJ/mol	Joback Method
hfus	35.36	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.990		Crippen Method
mcvol	232.860	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	660.37	K	Joback Method
tc	822.79	K	Joback Method
tf	369.80	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.09	J/mol×K	660.37	Joback Method
cpg	684.86	J/mol×K	687.44	Joback Method
cpg	696.86	J/mol×K	714.51	Joback Method
cpg	708.14	J/mol×K	741.58	Joback Method
cpg	718.74	J/mol×K	768.65	Joback Method
cpg	728.70	J/mol×K	795.72	Joback Method
cpg	738.06	J/mol×K	822.79	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=U390702&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