Succinic acid, 3-methylbut-2-en-1-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C12H15F5O4/c1-8(2)5-6-20-9(18)3-4-10(19)21-7-11(13,14)12(15,16)17/h5H,3

InchiKey: WVOSARPQJOXUNG-UHFFFAOYSA-N

Formula: C12H15F5O4

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

Mol. weight [g/mol]: 318.24

Physical Properties

Property code	Value	Unit	Source
gf	-1314.38	kJ/mol	Joback Method
hf	-1671.23	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.017		Crippen Method
mcvol	199.370	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1362.00		NIST Webbook
rinpol	1362.00		NIST Webbook
tb	620.47	K	Joback Method
tc	789.43	K	Joback Method
tf	358.07	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.39	J/mol×K	620.47	Joback Method
cpg	553.92	J/mol×K	648.63	Joback Method
cpg	565.76	J/mol×K	676.79	Joback Method
cpg	576.92	J/mol×K	704.95	Joback Method
cpg	587.43	J/mol×K	733.11	Joback Method
cpg	597.34	J/mol×K	761.27	Joback Method
cpg	606.66	J/mol×K	789.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390863&Units=SI

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