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

Inchi: InChI=1S/C12H16F4O4/c1-8(2)5-6-19-9(17)3-4-10(18)20-7-12(15,16)11(13)14/h5,11H,3

InchiKey: RPCFVTMENNLDHY-UHFFFAOYSA-N

Formula: C12H16F4O4

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

Mol. weight [g/mol]: 300.25

Physical Properties

Property code	Value	Unit	Source
gf	-1124.85	kJ/mol	Joback Method
hf	-1471.65	kJ/mol	Joback Method
hfus	32.68	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.720		Crippen Method
mcvol	197.600	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	623.99	K	Joback Method
tc	794.41	K	Joback Method
tf	340.06	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.59	J/mol×K	623.99	Joback Method
cpg	543.40	J/mol×K	652.39	Joback Method
cpg	555.56	J/mol×K	680.80	Joback Method
cpg	567.07	J/mol×K	709.20	Joback Method
cpg	577.96	J/mol×K	737.60	Joback Method
cpg	588.26	J/mol×K	766.01	Joback Method
cpg	597.97	J/mol×K	794.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390850&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