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

Inchi: InChI=1S/C12H17F3O4/c1-8(2)6-7-18-10(16)4-5-11(17)19-9(3)12(13,14)15/h6,9H,4-5,7H

InchiKey: PZVQCFMVKBPXAS-UHFFFAOYSA-N

Formula: C12H17F3O4

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

Mol. weight [g/mol]: 282.26

Physical Properties

Property code	Value	Unit	Source
gf	-930.04	kJ/mol	Joback Method
hf	-1275.54	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.770		Crippen Method
mcvol	195.830	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
tb	624.72	K	Joback Method
tc	801.34	K	Joback Method
tf	339.47	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/mol×K	624.72	Joback Method
cpg	535.83	J/mol×K	654.16	Joback Method
cpg	548.45	J/mol×K	683.59	Joback Method
cpg	560.39	J/mol×K	713.03	Joback Method
cpg	571.68	J/mol×K	742.47	Joback Method
cpg	582.33	J/mol×K	771.90	Joback Method
cpg	592.37	J/mol×K	801.34	Joback Method

Sources

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=U390841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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