Succinic acid, 1,1,1-trifluoroprop-2-yl 3-methylbut-3-en-1-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/h9H,1,4-7H2

InchiKey: TZBDGRBURWLXSE-UHFFFAOYSA-N

Formula: C12H17F3O4

SMILES: C=C(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	-922.42	kJ/mol	Joback Method
hf	-1267.33	kJ/mol	Joback Method
hfus	28.12	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.770		Crippen Method
mcvol	195.830	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
tb	617.24	K	Joback Method
tc	790.50	K	Joback Method
tf	342.79	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.66	J/mol×K	617.24	Joback Method
cpg	534.93	J/mol×K	646.12	Joback Method
cpg	547.53	J/mol×K	674.99	Joback Method
cpg	559.48	J/mol×K	703.87	Joback Method
cpg	570.78	J/mol×K	732.75	Joback Method
cpg	581.47	J/mol×K	761.63	Joback Method
cpg	591.54	J/mol×K	790.50	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=U391128&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