Succinic acid, 1,1,1-trifluoroprop-2-yl cis-hex-3-en-1-yl ester

Inchi: InChI=1S/C13H19F3O4/c1-3-4-5-6-9-19-11(17)7-8-12(18)20-10(2)13(14,15)16/h4-5,10H

InchiKey: KEMQJFHOIBOQSY-PLNGDYQASA-N

Formula: C13H19F3O4

SMILES: CCC=CCCOC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 296.28

Physical Properties

Property code	Value	Unit	Source
gf	-913.07	kJ/mol	Joback Method
hf	-1286.39	kJ/mol	Joback Method
hfus	33.50	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.160		Crippen Method
mcvol	209.920	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
tb	647.72	K	Joback Method
tc	821.37	K	Joback Method
tf	364.70	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	647.72	Joback Method
cpg	587.93	J/mol×K	676.66	Joback Method
cpg	600.92	J/mol×K	705.60	Joback Method
cpg	613.22	J/mol×K	734.55	Joback Method
cpg	624.85	J/mol×K	763.49	Joback Method
cpg	635.83	J/mol×K	792.43	Joback Method
cpg	646.20	J/mol×K	821.37	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=U391079&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