Succinic acid, 1,1,1-trifluoroprop-2-yl 2-methylpent-3-yl ester

Inchi: InChI=1S/C13H21F3O4/c1-5-10(8(2)3)20-12(18)7-6-11(17)19-9(4)13(14,15)16/h8-10H,5

InchiKey: YXTPRSCHDVIUQB-UHFFFAOYSA-N

Formula: C13H21F3O4

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

Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
gf	-998.17	kJ/mol	Joback Method
hf	-1414.17	kJ/mol	Joback Method
hfus	26.26	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.238		Crippen Method
mcvol	214.220	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
tb	642.68	K	Joback Method
tc	815.89	K	Joback Method
tf	339.78	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.47	J/mol×K	642.68	Joback Method
cpg	611.15	J/mol×K	671.55	Joback Method
cpg	625.09	J/mol×K	700.42	Joback Method
cpg	638.29	J/mol×K	729.29	Joback Method
cpg	650.78	J/mol×K	758.15	Joback Method
cpg	662.57	J/mol×K	787.02	Joback Method
cpg	673.68	J/mol×K	815.89	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=U389593&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