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

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

InchiKey: VFSATUKXHJPZMM-UHFFFAOYSA-N

Formula: C13H21F3O4

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

Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
gf	-992.89	kJ/mol	Joback Method
hf	-1417.64	kJ/mol	Joback Method
hfus	22.37	kJ/mol	Joback Method
hvap	57.03	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.238		Crippen Method
mcvol	214.220	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1341.00		NIST Webbook
tb	639.89	K	Joback Method
tc	817.70	K	Joback Method
tf	357.20	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.89	J/mol×K	639.89	Joback Method
cpg	613.80	J/mol×K	669.53	Joback Method
cpg	627.88	J/mol×K	699.16	Joback Method
cpg	641.16	J/mol×K	728.80	Joback Method
cpg	653.66	J/mol×K	758.43	Joback Method
cpg	665.43	J/mol×K	788.07	Joback Method
cpg	676.47	J/mol×K	817.70	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=U390614&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