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

Inchi: InChI=1S/C12H19F3O4/c1-7(2)8(3)18-10(16)5-6-11(17)19-9(4)12(13,14)15/h7-9H,5-6H2

InchiKey: HGCNFDUVWFSBAI-UHFFFAOYSA-N

Formula: C12H19F3O4

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

Mol. weight [g/mol]: 284.27

Physical Properties

Property code	Value	Unit	Source
gf	-1006.59	kJ/mol	Joback Method
hf	-1393.53	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.848		Crippen Method
mcvol	200.130	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1296.00		NIST Webbook
tb	619.80	K	Joback Method
tc	793.70	K	Joback Method
tf	328.51	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.39	J/mol×K	619.80	Joback Method
cpg	558.56	J/mol×K	648.78	Joback Method
cpg	572.02	J/mol×K	677.77	Joback Method
cpg	584.79	J/mol×K	706.75	Joback Method
cpg	596.87	J/mol×K	735.74	Joback Method
cpg	608.28	J/mol×K	764.72	Joback Method
cpg	619.03	J/mol×K	793.70	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=U390577&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