Succinic acid, 1,1,1-trifluoroprop-2-yl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C14H23F3O4/c1-8(2)13(9(3)4)21-12(19)7-6-11(18)20-10(5)14(15,16)17/h8-10

InchiKey: XSIGMHWSUFXFCF-UHFFFAOYSA-N

Formula: C14H23F3O4

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

Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-992.19	kJ/mol	Joback Method
hf	-1440.09	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	59.77	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.484		Crippen Method
mcvol	228.310	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	665.12	K	Joback Method
tc	840.30	K	Joback Method
tf	336.05	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.35	J/mol×K	665.12	Joback Method
cpg	665.73	J/mol×K	694.32	Joback Method
cpg	680.30	J/mol×K	723.51	Joback Method
cpg	694.08	J/mol×K	752.71	Joback Method
cpg	707.09	J/mol×K	781.91	Joback Method
cpg	719.34	J/mol×K	811.10	Joback Method
cpg	730.85	J/mol×K	840.30	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=U390498&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

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