Succinic acid, isohexyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C14H24O5/c1-10(2)6-5-9-18-13(16)7-8-14(17)19-12(4)11(3)15/h10,12H,5-9H2
InchiKey: RPFZHXUTUDRXQI-UHFFFAOYSA-N
Formula: C14H24O5
SMILES: CC(=O)C(C)OC(=O)CCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 272.34

Physical Properties

Property code	Value	Unit	Source
gf	-534.64	kJ/mol	Joback Method
hf	-945.03	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.267		Crippen Method
mcvol	224.570	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1781.00		NIST Webbook
tb	725.29	K	Joback Method
tc	913.53	K	Joback Method
tf	411.79	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.84	J/mol×K	725.29	Joback Method
cpg	659.70	J/mol×K	756.66	Joback Method
cpg	673.72	J/mol×K	788.04	Joback Method
cpg	686.91	J/mol×K	819.41	Joback Method
cpg	699.26	J/mol×K	850.78	Joback Method
cpg	710.79	J/mol×K	882.15	Joback Method
cpg	721.49	J/mol×K	913.53	Joback Method
dvisc	0.0016806	Pa×s	411.79	Joback Method

dvisc	0.0008061	Pa×s	464.04	Joback Method
dvisc	0.0004486	Pa×s	516.29	Joback Method
dvisc	0.0002781	Pa×s	568.54	Joback Method
dvisc	0.0001868	Pa×s	620.79	Joback Method
dvisc	0.0001335	Pa×s	673.04	Joback Method
dvisc	0.0001001	Pa×s	725.29	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U349580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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