Succinic acid, di(3-oxobut-2-yl) ester

Inchi: InChI=1S/C12H18O6/c1-7(13)9(3)17-11(15)5-6-12(16)18-10(4)8(2)14/h9-10H,5-6H2,1-4
InchiKey: MJFIYODJICINQS-UHFFFAOYSA-N
Formula: C12H18O6
SMILES: CC(=O)C(C)OC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-680.40	kJ/mol	Joback Method
hf	-1016.33	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.808		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
tb	733.40	K	Joback Method
tc	930.78	K	Joback Method
tf	439.18	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.68	J/mol×K	733.40	Joback Method
cpg	566.31	J/mol×K	766.30	Joback Method
cpg	578.13	J/mol×K	799.19	Joback Method
cpg	589.14	J/mol×K	832.09	Joback Method
cpg	599.33	J/mol×K	864.99	Joback Method
cpg	608.71	J/mol×K	897.88	Joback Method
cpg	617.27	J/mol×K	930.78	Joback Method
dvisc	0.0015495	Pa×s	439.18	Joback Method

dvisc	0.0008271	Pa×s	488.22	Joback Method
dvisc	0.0004951	Pa×s	537.25	Joback Method
dvisc	0.0003229	Pa×s	586.29	Joback Method
dvisc	0.0002250	Pa×s	635.33	Joback Method
dvisc	0.0001651	Pa×s	684.36	Joback Method
dvisc	0.0001263	Pa×s	733.40	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=U349590&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