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

Inchi: InChI=1S/C14H22O6/c1-9(15)11(3)19-13(17)7-5-6-8-14(18)20-12(4)10(2)16/h11-12H,5-8
InchiKey: DXBGSZKUGZQFII-UHFFFAOYSA-N
Formula: C14H22O6
SMILES: CC(=O)C(C)OC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 286.32

Physical Properties

Property code	Value	Unit	Source
gf	-663.56	kJ/mol	Joback Method
hf	-1057.61	kJ/mol	Joback Method
hfus	33.74	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.588		Crippen Method
mcvol	226.140	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
tb	779.16	K	Joback Method
tc	974.73	K	Joback Method
tf	461.72	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.46	J/mol×K	779.16	Joback Method
cpg	675.88	J/mol×K	811.76	Joback Method
cpg	688.40	J/mol×K	844.35	Joback Method
cpg	700.02	J/mol×K	876.95	Joback Method
cpg	710.73	J/mol×K	909.54	Joback Method
cpg	720.55	J/mol×K	942.14	Joback Method
cpg	729.46	J/mol×K	974.73	Joback Method
dvisc	0.0012786	Pa×s	461.72	Joback Method

dvisc	0.0006654	Pa×s	514.63	Joback Method
dvisc	0.0003911	Pa×s	567.53	Joback Method
dvisc	0.0002517	Pa×s	620.44	Joback Method
dvisc	0.0001736	Pa×s	673.35	Joback Method
dvisc	0.0001264	Pa×s	726.25	Joback Method
dvisc	0.0000961	Pa×s	779.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U353763&Units=SI

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