Acetoxyacetic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C9H16O4/c1-6(2)7(3)13-9(11)5-12-8(4)10/h6-7H,5H2,1-4H3
InchiKey: JALLQYLJDDRAFM-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: CC(=O)OCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
gf	-447.82	kJ/mol	Joback Method
hf	-729.25	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.137		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	557.02	K	Joback Method
tc	745.99	K	Joback Method
tf	305.51	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.76	J/mol×K	557.02	Joback Method
cpg	381.74	J/mol×K	588.51	Joback Method
cpg	394.19	J/mol×K	620.01	Joback Method
cpg	406.09	J/mol×K	651.50	Joback Method
cpg	417.44	J/mol×K	683.00	Joback Method
cpg	428.24	J/mol×K	714.49	Joback Method
cpg	438.48	J/mol×K	745.99	Joback Method
dvisc	0.0033834	Pa×s	305.51	Joback Method

dvisc	0.0015540	Pa×s	347.43	Joback Method
dvisc	0.0008440	Pa×s	389.35	Joback Method
dvisc	0.0005161	Pa×s	431.26	Joback Method
dvisc	0.0003443	Pa×s	473.18	Joback Method
dvisc	0.0002454	Pa×s	515.10	Joback Method
dvisc	0.0001840	Pa×s	557.02	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=U355698&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

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