Butanoic acid, 2-methyl-3-oxo-, methyl ester

Other names:	Acetoacetic acid, 2-methyl-, methyl ester
	Methyl «alpha»-methylacetoacetate
	Methyl 2-methyl-3-oxobutyrate
	methyl 2-methylacetoacetate
	methyl 2-methyl-3-oxobutanoate
Inchi:	InChI=1S/C6H10O3/c1-4(5(2)7)6(8)9-3/h4H,1-3H3
InchiKey:	NDTWZHURUDSPQV-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	COC(=O)C(C)C(C)=O
Mol. weight [g/mol]:	130.14
CAS:	17094-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-365.64	kJ/mol	Joback Method
hf	-529.83	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	44.46	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.384		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	466.40	K	Joback Method
tc	659.46	K	Joback Method
tf	264.47	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.20	J/mol×K	466.40	Joback Method
cpg	259.68	J/mol×K	627.28	Joback Method
cpg	251.53	J/mol×K	595.11	Joback Method
cpg	243.00	J/mol×K	562.93	Joback Method

cpg	234.10	J/mol×K	530.75	Joback Method
cpg	224.83	J/mol×K	498.58	Joback Method
cpg	267.46	J/mol×K	659.46	Joback Method
dvisc	0.0002994	Pa×s	466.40	Joback Method
dvisc	0.0003862	Pa×s	432.75	Joback Method
dvisc	0.0005201	Pa×s	399.09	Joback Method
dvisc	0.0007400	Pa×s	365.44	Joback Method
dvisc	0.0011308	Pa×s	331.78	Joback Method
dvisc	0.0019016	Pa×s	298.12	Joback Method
dvisc	0.0036503	Pa×s	264.47	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=C17094212&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume