Methyl acetoacetate

Other names:	3-Oxobutanoic acid methyl ester
	3-oxobutanoic acid, methyl ester
	Acetoacetic methyl ester
	Butanoic acid, 3-oxo-, methyl ester
	Methyl 3-oxobutyrate
	Methyl acetylacetate
	Methyl acetylacetonate
	Methylester kyseliny acetoctove
	acetoacetic acid, methyl ester
	methyl 3-oxobutanoate
Inchi:	InChI=1S/C5H8O3/c1-4(6)3-5(7)8-2/h3H2,1-2H3
InchiKey:	WRQNANDWMGAFTP-UHFFFAOYSA-N
Formula:	C5H8O3
SMILES:	COC(=O)CC(C)=O
Mol. weight [g/mol]:	116.12
CAS:	105-45-3

Physical Properties

Property code	Value	Unit	Source
chl	-2487.70	kJ/mol	NIST Webbook
gf	-371.62	kJ/mol	Joback Method
hf	-503.91	kJ/mol	Joback Method
hfl	-623.21	kJ/mol	NIST Webbook
hfus	13.09	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
ie	9.81	eV	NIST Webbook
log10ws	-0.06		Crippen Method
logp	0.138		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
ripol	1396.00		NIST Webbook
tb	443.96	K	Joback Method
tc	634.74	K	Joback Method
tf	241.25	K	NIST Webbook
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.41	J/mol×K	443.96	Joback Method
cpg	213.74	J/mol×K	602.95	Joback Method
cpg	206.83	J/mol×K	571.15	Joback Method
cpg	199.65	J/mol×K	539.35	Joback Method
cpg	192.17	J/mol×K	507.55	Joback Method
cpg	184.43	J/mol×K	475.76	Joback Method
cpg	220.34	J/mol×K	634.74	Joback Method
dvisc	0.0015356	Pa×s	297.49	Joback Method
dvisc	0.0010084	Pa×s	326.79	Joback Method
dvisc	0.0007096	Pa×s	356.08	Joback Method
dvisc	0.0005268	Pa×s	385.37	Joback Method
dvisc	0.0004079	Pa×s	414.67	Joback Method
dvisc	0.0003266	Pa×s	443.96	Joback Method
dvisc	0.0025634	Pa×s	268.20	Joback Method
hvapt	45.40	kJ/mol	367.50	NIST Webbook
rhol	1081.93	kg/m3	288.20	Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa
rhol	1016.95	kg/m3	348.20	Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa

rhol	1027.89	kg/m3	338.20	Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa	
rhol	1038.78	kg/m3	328.20	Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa	
rhol	1055.01	kg/m3	313.20	Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa	
rhol	1071.18	kg/m3	298.20	Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at T = (288.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa	
srf	0.04	N/m	298.15	Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Organic Non-Electrolytes	

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105453&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solute-Solvent Interactions of Alkyl Acetoacetates in Aqueous Concentration Dependence of Surface Tension for Very Dilute Aqueous Solutions of Non-Electrolytes:	https://www.doi.org/10.1016/j.tca.2013.12.015
1-Butyl-3-methylimidazolium Bromide [bmim][Br] Ionic Liquid Solutions in the Temperature Interval (288.15 - 308.15) K:	https://www.doi.org/10.1021/je049955d
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solute Solvent Interactions of Alkyl Acetoacetates in Aqueous [1-Butyl-3-methylimidazolium Chloride [bmim][Cl] Ionic Liquid Solutions in the Temperature Interval (288.15 - 308.15) K:	https://www.doi.org/10.1021/je4009987
Excess Molar Enthalpies of Methyl Acetoacetate + (Methanol, + Ethanol, + 1-Propanol, + 2-Propanol) at T = (298.2, 298.2, 313.2, and 328.2) K and p = 101.3 kPa :	https://www.doi.org/10.1021/je1006482
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume