Ethyl acetoacetate

Other names:	1-Ethoxybutane-1,3-dione
	3-Oxobutanoic acid ethyl ester
	3-oxobutanoic acid, ethyl ester
	Acetoacetic acid, ethyl ester
	Acetoctan ethylnaty
	Active acetylacetate
	Butanoic acid, 3-oxo-, ethyl ester
	Diacetic ether
	EAA
	Ethyl 3-oxobutanoate
	Ethyl 3-oxobutyrate
	Ethyl acetylacetate
	Ethylacetacetat
	Ethylester kyseliny acetoctove
	NSC 8657
	acetoacetic acid ethyl ester
	ethyl 3-ketobutyrate
	ethyl acetonecarboxylate
Inchi:	InChI=1S/C6H10O3/c1-3-9-6(8)4-5(2)7/h3-4H2,1-2H3
InchiKey:	XYIBRDXRRQCHLP-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CCOC(=O)CC(C)=O
Mol. weight [g/mol]:	130.14
CAS:	141-97-9

Physical Properties

Property code	Value	Unit	Source
chl	-3149.76 ± 0.76	kJ/mol	NIST Webbook
chl	-3178.10 ± 7.70	kJ/mol	NIST Webbook
chl	-3153.00	kJ/mol	NIST Webbook
gf	-363.20	kJ/mol	Joback Method
hf	-558.00	kJ/mol	NIST Webbook
hf	-507.50	kJ/mol	NIST Webbook
hf	-586.20 ± 1.50	kJ/mol	NIST Webbook
hfl	-561.70	kJ/mol	NIST Webbook
hfl	-612.20 ± 5.40	kJ/mol	NIST Webbook
hfl	-640.40 ± 1.10	kJ/mol	NIST Webbook

hfus	15.68	kJ/mol	Joback Method
hvap	54.18 ± 0.96	kJ/mol	NIST Webbook
hvap	54.20 ± 1.00	kJ/mol	NIST Webbook
hvap	54.20	kJ/mol	NIST Webbook
hvap	50.54	kJ/mol	NIST Webbook
log10ws	-0.48		Crippen Method
logp	0.529		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	907.00		NIST Webbook
rinpol	944.40		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	910.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1496.00		NIST Webbook
tb	466.84	K	Joback Method
tc	655.65	K	Joback Method
tf	230.15	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.00	J/mol×K	466.84	Joback Method
cpg	224.34	J/mol×K	498.31	Joback Method
cpg	233.35	J/mol×K	529.78	Joback Method
cpg	242.00	J/mol×K	561.25	Joback Method
cpg	250.31	J/mol×K	592.71	Joback Method
cpg	258.27	J/mol×K	624.18	Joback Method
cpg	265.88	J/mol×K	655.65	Joback Method
cpl	250.20	J/mol×K	297.50	NIST Webbook
cpl	246.90	J/mol×K	297.50	NIST Webbook
cpl	241.80	J/mol×K	298.00	NIST Webbook

dvisc	0.0019020	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0015810	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0013440	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0011440	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K

hvapt	61.60	kJ/mol	298.15	Thermochemistry of Ethyl 3-Oxobutanoate Revisited: Observance of a Non-Zero Enthalpy of Mixing between Tautomers and Its Effects on Enthalpies of Formation	
hvapt	52.50	kJ/mol	377.50	NIST Webbook	
rfi	1.41660		298.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K	
rfi	1.41200		308.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K	
rfi	1.41450		303.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dioctyl Phthalate at 298.15, 303.15, and 308.15 K	

rhol	1043.10	kg/m3	278.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa
rhol	1034.50	kg/m3	288.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa
rhol	1023.50	kg/m3	298.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa
rhol	1008.00	kg/m3	313.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa
rhol	992.10	kg/m3	328.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa

rhol	981.90	kg/m3	338.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa	
rhol	971.40	kg/m3	348.15	Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa	
rhol	1023.45	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K	
srf	0.03	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.03	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	

srf	0.03	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	347.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.07456e+01
Coeff. B	-7.62332e+03
Coeff. C	-4.83240e+00
Coeff. D	1.05324e-06
Temperature range (K), min.	234.15
Temperature range (K), max.	643.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141979&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of 1,4-Dioxane + Ethyl Acetoacetate, + Diethyl Oxalate, + Diethyl Phthalate, or + Dibutyl Phthalate at 298.15, 303.15, and 308.15 K:	https://www.doi.org/10.1021/je0301489
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Binary Mixtures from T = 288.15 K to T = 318.15 K: Solute-Solvent Interactions of Alkyl Acetoacetates in Aqueous (1-Butyl-3-methylimidazolium Bromide + Ionic Liquid) Solutions	https://www.doi.org/10.1021/je050170x
Thermochemistry of Ethyl 3-Oxobutanoate Revisited: Observance of Enthalpy–Entropy Compensation	https://www.cheric.org/files/research/kdb/mol/mol1072.mol
Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate + Ethanol, + 1-Propanol, and + 2-Propanol at T = (298.15, 313.15, and 328.15) K	https://www.doi.org/10.1016/j.tca.2013.12.015
Solvent Effects on Enthalpies of Dilution: Excess Molar Enthalpies of Binary Mixtures Containing Ethyl Acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa	https://www.doi.org/10.1021/je050179z
Densities, Viscosities, Refractive Indices, and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate + Ethanol at (288.15, 298.15, 308.15, and 318.15) K	https://www.doi.org/10.1021/je060139a
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Solute–Solvent Interactions of Alkyl Salicylate, and Benzyl Propionate with Ethanol at 298.15, 308.15, and 318.15 K	https://www.doi.org/10.1021/je4009987
Excess Molar Enthalpies of Binary Mixtures of 1-Methylimidazolium Chloride Ionic Liquid Solutions in the Temperature Interval 288.15 K to 318.15 K	https://www.doi.org/10.1021/je800889y
Excess molar enthalpies of ethyl acetoacetate + (methanol, +ethanol, +1-propanol, and +2-propanol) at T = (298.15, 313.15 and 328.15)K and p = (0.1 and 10.0)MPa.	https://www.doi.org/10.1016/j.fluid.2008.03.012
KDB: Vapor Pressure Data	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1072
Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je050402s

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume