Butanoic acid, 3-methyl-, ethyl ester

Other names:	(CH3)2CHCH2C(O)OC2H5
	3-Methylbutanoic acid ethyl ester
	3-methyl butyric acid ethyl ester
	3-methylbutanoic acid, ethyl ester
	Butyric acid, 3-methyl-, ethyl ester
	ETHYL 3-METHYLBUTYRATE
	ETHYL ESTER ISOVALERIC ACID
	ETHYL ISO-PENTANOATE
	Ethyl 3-methylbutanoate
	Ethyl isovalerate
	Isovaleric acid, ethyl ester
	ethyl 3-methylbutanoate (ethyl isovalerate)
Inchi:	InChI=1S/C7H14O2/c1-4-9-7(8)5-6(2)3/h6H,4-5H2,1-3H3
InchiKey:	PPXUHEORWJQRHJ-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCOC(=O)CC(C)C
Mol. weight [g/mol]:	130.18
CAS:	108-64-5

Physical Properties

Property code	Value	Unit	Source
chl	-4184.40 ± 8.40	kJ/mol	NIST Webbook
gf	-228.30	kJ/mol	Joback Method
hf	-527.20 ± 8.80	kJ/mol	NIST Webbook
hfl	-571.30 ± 8.40	kJ/mol	NIST Webbook
hfus	13.15	kJ/mol	Joback Method
hvap	44.10	kJ/mol	NIST Webbook
hvap	44.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	848.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	852.00		NIST Webbook

rinpol	851.00	NIST Webbook
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rinpol	860.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	855.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	838.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	849.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	855.00	NIST Webbook
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ripol	1080.00		NIST Webbook
ripol	1088.00		NIST Webbook
ripol	1096.00		NIST Webbook
tb	407.90	K	NIST Webbook
tb	405.20	K	NIST Webbook
tb	407.90 ± 0.50	K	NIST Webbook
tb	407.90 ± 0.50	K	NIST Webbook
tb	408.55 ± 0.40	K	NIST Webbook
tc	588.02 ± 6.00	K	NIST Webbook
tc	582.40 ± 0.60	K	NIST Webbook
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
dvisc	0.0006590	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005440	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005810	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0006200	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0005160	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0004850	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0004570	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0004310	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0008530	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	0.0007390	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	0.0006420	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	0.0008050	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0007520	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0007030	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters	
dvisc	0.0005660	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	44.50	kJ/mol	337.00	NIST Webbook	
hvapt	42.80	kJ/mol	359.50	NIST Webbook	

rhol	859.78	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	0.02	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
srf	0.02	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	0.02	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	0.02	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	0.02	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	0.02	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	0.02	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	0.02	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.26655e+01
Coeff. B	-7.05868e+03
Coeff. C	-6.91517e+00
Coeff. D	4.16650e-06
Temperature range (K), min.	173.85
Temperature range (K), max.	587.95

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1087
Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters:	https://www.doi.org/10.1021/je050001c
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K:	https://www.doi.org/10.1021/je050170x
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1087.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108645&Units=SI
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:	https://www.doi.org/10.1021/je060139a

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume