

Methyl valerate

Other names:	CH ₃ (CH ₂) ₃ COOCH ₃ Methyl ester of pentanoic acid Methyl n-valerate Methyl pentanoate Methyl valerianate Pentanoic acid, methyl ester Propyl propanoate Valeric acid, methyl ester n-Valeric acid methyl ester valeric acid methyl ester
Inchi:	InChI=1S/C6H12O2/c1-3-4-5-6(7)8-2/h3-5H2,1-2H3
InchiKey:	HNBDRPTVWVGKBR-UHFFFAOYSA-N
Formula:	C ₆ H ₁₂ O ₂
SMILES:	CCCCC(=O)OC
Mol. weight [g/mol]:	116.16
CAS:	624-24-8

Physical Properties

Property code	Value	Unit	Source
chl	-3548.00	kJ/mol	NIST Webbook
chl	-3561.70 ± 0.60	kJ/mol	NIST Webbook
gf	-234.28	kJ/mol	Joback Method
hf	-485.00 ± 2.00	kJ/mol	NIST Webbook
hf	-472.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-527.00	kJ/mol	NIST Webbook
hfl	-514.20 ± 7.10	kJ/mol	NIST Webbook
hfus	14.08	kJ/mol	Joback Method
hvap	38.11	kJ/mol	Joback Method
ie	10.40 ± 0.20	eV	NIST Webbook
log10ws	-1.34		Estimated Solubility Method
log10ws	-1.36		Aqueous Solubility Prediction Method
logp	1.350		Crippen Method
mvol	102.840	ml/mol	McGowan Method
pc	3190.00 ± 202.65	kPa	NIST Webbook
rhoc	278.78 ± 19.75	kg/m ³	NIST Webbook

rinpol	808.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	804.00	NIST Webbook
rinpol	808.80	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	809.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	829.10	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	808.80	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	806.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	830.00	NIST Webbook

ripol	802.00		NIST Webbook
ripol	794.00		NIST Webbook
ripol	821.20		NIST Webbook
ripol	822.80		NIST Webbook
ripol	822.80		NIST Webbook
ripol	821.90		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1083.00		NIST Webbook
tb	400.48	K	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
tc	566.90 ± 20.00	K	NIST Webbook
tc	556.70 ± 20.00	K	NIST Webbook
tf	182.50 ± 0.05	K	NIST Webbook
vc	0.396	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.38	J/mol×K	531.36	Joback Method

cpg	209.71	J/molxK	442.57	Joback Method
cpg	254.27	J/molxK	590.55	Joback Method
cpg	245.98	J/molxK	560.96	Joback Method
cpg	219.25	J/molxK	472.16	Joback Method
cpg	228.47	J/molxK	501.76	Joback Method
cpg	199.87	J/molxK	412.97	Joback Method
cpl	226.11	J/molxK	298.15	NIST Webbook
cpl	229.30	J/molxK	298.15	NIST Webbook
dvisc	0.0007120	Paxs	293.15	A Study on Properties Derived from Densities and Viscosities for the Ternary Systems (Methyl Pentanoate or Methyl Heptanoate) + n-Octane + 1-Hexanol and their Binary Subsystems at Various Temperatures.
dvisc	0.0006610	Paxs	298.15	A Study on Properties Derived from Densities and Viscosities for the Ternary Systems (Methyl Pentanoate or Methyl Heptanoate) + n-Octane + 1-Hexanol and their Binary Subsystems at Various Temperatures.
dvisc	0.0006230	Paxs	303.15	A Study on Properties Derived from Densities and Viscosities for the Ternary Systems (Methyl Pentanoate or Methyl Heptanoate) + n-Octane + 1-Hexanol and their Binary Subsystems at Various Temperatures.

dvisc	0.0005510	Paxs	313.15	A Study on Properties Derived from Densities and Viscosities for the Ternary Systems (Methyl Pentanoate or Methyl Heptanoate) + n-Octane + 1-Hexanol and their Binary Subsystems at Various Temperatures.
dvisc	0.0008160	Paxs	283.15	A Study on Properties Derived from Densities and Viscosities for the Ternary Systems (Methyl Pentanoate or Methyl Heptanoate) + n-Octane + 1-Hexanol and their Binary Subsystems at Various Temperatures.
hvapt	44.40	kJ/mol	414.00	NIST Webbook
hvapt	42.50	kJ/mol	354.00	NIST Webbook
hvapt	44.10 ± 0.10	kJ/mol	382.50	NIST Webbook
hvapt	41.30	kJ/mol	350.00	NIST Webbook
hvapt	39.20	kJ/mol	390.50	NIST Webbook
pvap	1.58	kPa	299.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.87	kPa	289.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.93	kPa	290.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	1.03	kPa	292.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.09	kPa	293.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.13	kPa	293.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.23	kPa	294.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.33	kPa	296.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.51	kPa	297.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.52	kPa	298.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.61	kPa	299.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.83	kPa	288.70	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	1.97	kPa	302.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.94	kPa	302.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.27	kPa	305.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.65	kPa	308.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	3.11	kPa	311.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	101.30	kPa	400.48	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	100.40	kPa	400.07	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	95.08	kPa	398.03	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	88.17	kPa	395.42	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane

pvap	77.71	kPa	391.14	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	0.82	kPa	288.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	59.35	kPa	382.55	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	52.83	kPa	378.84	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	45.81	kPa	374.53	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	40.47	kPa	370.86	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	35.06	kPa	366.70	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	29.41	kPa	361.82	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	60.00	kPa	383.29	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	0.78	kPa	288.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.79	kPa	288.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.75	kPa	287.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.69	kPa	285.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.62	kPa	284.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.60	kPa	284.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.64	kPa	284.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.52	kPa	281.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.46	kPa	279.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.34	kPa	275.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.34	kPa	274.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.42	kPa	278.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	69.02	kPa	387.18	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	0.56	kPa	282.60	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
rfi	1.39500		298.15	Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV: Hex and Vex for 25 binary mixtures $\{xC(u-1)H(2u-1)CO_2CH_3 + (1-x)\alpha,\omega\text{-BrCH}_2(\text{CH}_2)(v-2)\text{CH}_2\text{Br}\}$, where $u = 1$ to 5 , $\alpha = 1$ and $v = \omega = 2$ to 6
rfi	1.39520		298.15	Mixing thermodynamic properties of ester-containing solutions: A study on the ternary (methyl alkanoate (pentanoate and methanoate) + methanol) and the corresponding binaries. New contributions to the (ester + ester) interactions

rfi	1.39680		298.15	A Study on Alkane + Ester + Ester Systems. Physicochemical Behavior of Binaries and Ternaries of Octane or Iso-octane with Methyl Esters (Ethanoate, Butanoate, Pentanoate)
rfi	1.39470		298.15	Isobaric Vapor-Liquid Equilibria and Excess Properties for the Binary Systems of Methyl Esters + Heptane
rfi	1.39710		298.15	Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Acetonitrile (2) Systems at 93.32 kPa
rfi	1.39710		298.15	Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Propanenitrile (2) Systems at 93.32 kPa
rhoI	885.66	kg/m ³	298.15	Densities and interfacial tensions for fatty acid methyl esters (from methyl formate to methyl heptanoate) + water demixed mixtures at atmospheric pressure conditions
tcondI	0.14	W/m×K	295.51	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.14	W/m×K	298.99	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	305.50	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	290.39	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	285.55	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	312.35	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	362.16	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	355.39	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.12	W/m×K	348.36	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	340.41	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	333.50	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	327.35	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	320.42	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40423e+01
Coeff. B	-3.36903e+03
Coeff. C	-5.25030e+01
Temperature range (K), min.	297.44

Temperature range (K), max.	438.38
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Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.06981e+02
Coeff. B	-8.88364e+03
Coeff. C	-1.35161e+01
Coeff. D	6.94116e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	575.15

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
293.15	100.00	890.18
293.15	1000.00	890.39
293.15	3000.00	892.23
293.15	5000.00	893.59
293.15	10000.00	897.77
293.15	15000.00	901.59
293.15	20000.00	905.28
293.15	25000.00	908.91
293.15	30000.00	912.4
293.15	35000.00	915.63
293.15	40000.00	918.78
293.15	50000.00	925.12
293.15	60000.00	930.63
303.15	100.00	879.57
303.15	1000.00	880.52
303.15	3000.00	882.29
303.15	5000.00	884.05
303.15	10000.00	888.3
303.15	15000.00	892.37
303.15	20000.00	896.14
303.15	25000.00	899.89

303.15	30000.00	903.55
303.15	35000.00	906.97
303.15	40000.00	910.27
303.15	50000.00	916.73
303.15	60000.00	922.74
313.15	100.00	869.49
313.15	1000.00	869.89
313.15	3000.00	871.87
313.15	5000.00	873.76
313.15	10000.00	878.33
313.15	15000.00	882.44
313.15	20000.00	886.62
313.15	25000.00	890.61
313.15	30000.00	894.38
313.15	35000.00	898.09
313.15	40000.00	901.45
313.15	50000.00	908.24
313.15	60000.00	914.32
323.15	100.00	858.83
323.15	1000.00	859.81
323.15	3000.00	861.81
323.15	5000.00	863.85
323.15	10000.00	868.67
323.15	15000.00	873.18
323.15	20000.00	877.67
323.15	25000.00	881.64
323.15	30000.00	885.65
323.15	35000.00	889.44
323.15	40000.00	893.13
323.15	50000.00	900.12
323.15	60000.00	906.77
333.15	100.00	848.52
333.15	1000.00	849.45
333.15	3000.00	851.71
333.15	5000.00	853.79
333.15	10000.00	858.86
333.15	15000.00	863.66
333.15	20000.00	868.26
333.15	25000.00	872.72
333.15	30000.00	876.79
333.15	35000.00	880.79
333.15	40000.00	884.78
333.15	50000.00	892.02
333.15	60000.00	898.8

343.15	100.00	837.8
343.15	1000.00	839.04
343.15	3000.00	841.41
343.15	5000.00	843.76
343.15	10000.00	849.05
343.15	15000.00	854.23
343.15	20000.00	859.25
343.15	25000.00	863.69
343.15	30000.00	868.17
343.15	35000.00	872.41
343.15	40000.00	876.28
343.15	50000.00	884.03
343.15	60000.00	890.84
353.15	100.00	827.35
353.15	1000.00	828.43
353.15	3000.00	831.13
353.15	5000.00	833.48
353.15	10000.00	839.27
353.15	15000.00	844.84
353.15	20000.00	849.86
353.15	25000.00	854.79
353.15	30000.00	859.45
353.15	35000.00	863.9
353.15	40000.00	868.0
353.15	50000.00	875.94
353.15	60000.00	883.37
363.15	100.00	816.63
363.15	1000.00	817.89
363.15	3000.00	820.7
363.15	5000.00	823.32
363.15	10000.00	829.23
363.15	15000.00	835.46
363.15	20000.00	840.59
363.15	25000.00	845.61
363.15	30000.00	850.57
363.15	35000.00	855.31
363.15	40000.00	859.8
363.15	50000.00	868.09
363.15	60000.00	875.9

Reference

<https://www.doi.org/10.1016/j.fluid.2018.04.024>

Sources

Vapor-Liquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Acetonitrile (2) Systems at 93.32 kPa: The Yaws Handbook of Vapor Pressure: Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel: Transpiration method: Vapor pressures and enthalpies of vaporization of some low boiling organic liquid densities of fatty acid methyl esters: Measurement and prediction with the PC-SAFT equation of state for ionic liquids. 8. Activity Coefficients and Equilibrium Measurements for the Carbonic Acid Esters and Aldehydes in 1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide Hexanoate, and Hexanoate (1) + Propanenitrile (2) Systems at 93.32 kPa: Experimental Study of the Thermodynamic Properties of Mixtures Containing Ionic Liquid Ethyl Sulfate Using Gas-Liquid Equilibrium and Transpiration Methods: Thermodynamic Properties of Binary and Ternary Mixtures of Ethyl Sulfate with Hydrocarbons, Alcohols, Esters, and Aldehydes in: Densities and Viscosities for the Binary and Ternary Mixtures of Methyl Pentanoate or Methyl Heptanoate with Octane, n-Heptane, and Ethyl Sulfate and their Binary Subsystems at Various Temperatures: Physical Behavior of Binaries and Ternaries of Octane or Iso-octane with Methyl Esters (Ethanoate, Butanoate, Pentanoate):

<https://www.doi.org/10.1021/je060001s>
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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<https://www.doi.org/10.1021/je034017j>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>
<https://www.doi.org/10.1021/acs.jced.5b00813>

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

ie:	Ionization energy
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
rhoc:	Critical density
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume

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