

Heptanoic acid, methyl ester

Other names:	Methyl enanthate Methyl ester of heptanoic acid Methyl heptanoate Methyl heptoate Methyl n-heptanoate Methyl n-heptylate Methyl oenanthylate enanthic acid, methyl ester methyl oenanthate oenanthic acid, methyl ester
Inchi:	InChI=1S/C8H16O2/c1-3-4-5-6-7-8(9)10-2/h3-7H2,1-2H3
InchiKey:	XNCNNDVCAUWAIT-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCCCC(=O)OC
Mol. weight [g/mol]:	144.21
CAS:	106-73-0

Physical Properties

Property code	Value	Unit	Source
chl	-4867.40 ± 0.80	kJ/mol	NIST Webbook
gf	-217.44	kJ/mol	Joback Method
hf	-517.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-567.10 ± 0.92	kJ/mol	NIST Webbook
hfus	19.26	kJ/mol	Joback Method
hvap	53.10 ± 0.10	kJ/mol	NIST Webbook
hvap	49.70 ± 0.50	kJ/mol	NIST Webbook
hvap	53.10 ± 0.40	kJ/mol	NIST Webbook
hvap	53.50	kJ/mol	NIST Webbook
hvap	51.62 ± 0.48	kJ/mol	NIST Webbook
hvap	51.60 ± 0.50	kJ/mol	NIST Webbook
hvap	50.00 ± 1.00	kJ/mol	NIST Webbook
hvap	50.10	kJ/mol	NIST Webbook
hvap	53.70	kJ/mol	NIST Webbook
hvap	53.40	kJ/mol	NIST Webbook
hvap	51.80 ± 0.10	kJ/mol	NIST Webbook
hvap	53.20 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.03		Crippen Method

logp	2.130		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	164.60		NIST Webbook
rinpol	164.60		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1023.90		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1023.90		NIST Webbook
rinpol	1023.30		NIST Webbook
rinpol	1022.90		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1008.60		NIST Webbook
rinpol	1008.10		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1027.70		NIST Webbook

ripol	1028.40		NIST Webbook
ripol	1013.00		NIST Webbook
ripol	1005.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1006.00		NIST Webbook
ripol	1006.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1273.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1273.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1273.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1241.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1291.00		NIST Webbook
tb	445.20	K	NIST Webbook
tb	446.95 ± 0.30	K	NIST Webbook
tb	445.30 ± 2.00	K	NIST Webbook
tc	633.80	K	Joback Method
tf	217.40 ± 0.50	K	NIST Webbook
tf	217.40 ± 0.05	K	NIST Webbook
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.10	J/mol×K	575.44	Joback Method
cpg	336.64	J/mol×K	604.62	Joback Method
cpg	291.94	J/mol×K	487.91	Joback Method
cpg	279.70	J/mol×K	458.73	Joback Method
cpg	346.77	J/mol×K	633.80	Joback Method
cpg	303.75	J/mol×K	517.09	Joback Method
cpg	315.14	J/mol×K	546.26	Joback Method
cpl	312.80	J/mol×K	363.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	289.20	J/mol×K	303.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	292.50	J/mol×K	313.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	296.20	J/mol×K	323.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	285.10	J/mol×K	298.15	NIST Webbook
cpl	300.10	J/mol×K	333.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	304.30	J/mol×K	343.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	308.60	J/mol×K	353.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters

cpl	316.90	J/molxK	373.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
dvisc	0.0010230	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	0.0008230	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	0.0009500	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	0.0013200	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.
dvisc	0.0011120	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.
hvapt	50.20 ± 0.10	kJ/mol	326.00	NIST Webbook
hvapt	49.00	kJ/mol	367.00	NIST Webbook
hvapt	49.10	kJ/mol	350.00	NIST Webbook
hvapt	46.30	kJ/mol	432.50	NIST Webbook
pvap	0.12	kPa	293.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.14	kPa	296.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.47	kPa	313.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.38	kPa	310.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.33	kPa	308.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.28	kPa	306.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.23	kPa	303.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.19	kPa	300.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.09	kPa	290.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.08	kPa	288.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.07	kPa	286.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.05	kPa	283.50	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.16	kPa	298.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.03	kPa	278.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
rfi	1.38724		348.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40945		298.15	Densities, speeds of sound, and refractive indices of the ternary mixtures (toluene + methyl acetate + butyl acetate) and (toluene + methyl acetate + methyl heptanoate) at 298.15 K
rfi	1.40945		298.15	Isobaric Vapor-Liquid Equilibria for the Binary Systems Benzene + Methyl Ethanoate, Benzene + Butyl Ethanoate, and Benzene + Methyl Heptanoate at 101.31kPa
rfi	1.38276		358.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38501		353.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38946		343.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39167		338.15	Thermophysical properties of fatty acid methyl and ethyl esters

rfi	1.39389		333.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39614		328.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39841		323.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40070		318.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40530		308.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40753		303.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40976		298.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41199		293.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41421		288.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41643		283.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41865		278.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40301		313.15	Thermophysical properties of fatty acid methyl and ethyl esters
rhol	875.61	kg/m3	298.15	Densities and interfacial tensions for fatty acid methyl esters (from methyl formate to methyl heptanoate) + water demixed mixtures at atmospheric pressure conditions

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51732e+01
Coeff. B	-4.00813e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	334.72
Temperature range (K), max.	471.89

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
293.15	100.00	880.16
293.15	1000.00	880.29
293.15	3000.00	881.98
293.15	5000.00	883.19
293.15	10000.00	886.99
293.15	15000.00	890.49
293.15	20000.00	893.86
293.15	25000.00	897.18
293.15	30000.00	900.36
293.15	35000.00	903.34
293.15	40000.00	906.22
293.15	50000.00	912.14
293.15	60000.00	917.16
303.15	100.00	870.66
303.15	1000.00	871.46
303.15	3000.00	873.07
303.15	5000.00	874.66
303.15	10000.00	878.5
303.15	15000.00	882.18

303.15	20000.00	885.64
303.15	25000.00	889.08
303.15	30000.00	892.3
303.15	35000.00	895.46
303.15	40000.00	898.49
303.15	50000.00	904.43
303.15	60000.00	909.95
313.15	100.00	861.82
313.15	1000.00	862.16
313.15	3000.00	863.9
313.15	5000.00	865.62
313.15	10000.00	869.71
313.15	15000.00	873.55
313.15	20000.00	877.29
313.15	25000.00	880.89
313.15	30000.00	884.32
313.15	35000.00	887.66
313.15	40000.00	890.73
313.15	50000.00	896.98
313.15	60000.00	902.59
323.15	100.00	852.25
323.15	1000.00	853.12
323.15	3000.00	854.89
323.15	5000.00	856.64
323.15	10000.00	860.97
323.15	15000.00	865.07
323.15	20000.00	869.08
323.15	25000.00	872.69
323.15	30000.00	876.31
323.15	35000.00	879.74
323.15	40000.00	883.15
323.15	50000.00	889.53
323.15	60000.00	895.63
333.15	100.00	843.03
333.15	1000.00	843.81
333.15	3000.00	845.84
333.15	5000.00	847.68
333.15	10000.00	852.16
333.15	15000.00	856.43
333.15	20000.00	860.63
333.15	25000.00	864.64
333.15	30000.00	868.31
333.15	35000.00	871.91
333.15	40000.00	875.61

333.15	50000.00	882.2
333.15	60000.00	888.39
343.15	100.00	833.48
343.15	1000.00	834.64
343.15	3000.00	836.7
343.15	5000.00	838.79
343.15	10000.00	843.47
343.15	15000.00	848.02
343.15	20000.00	852.59
343.15	25000.00	856.55
343.15	30000.00	860.57
343.15	35000.00	864.43
343.15	40000.00	867.96
343.15	50000.00	875.0
343.15	60000.00	881.19
353.15	100.00	824.35
353.15	1000.00	825.27
353.15	3000.00	827.61
353.15	5000.00	829.66
353.15	10000.00	834.76
353.15	15000.00	839.63
353.15	20000.00	844.11
353.15	25000.00	848.48
353.15	30000.00	852.65
353.15	35000.00	856.65
353.15	40000.00	860.37
353.15	50000.00	867.57
353.15	60000.00	874.32
363.15	100.00	815.19
363.15	1000.00	816.36
363.15	3000.00	818.75
363.15	5000.00	821.0
363.15	10000.00	826.14
363.15	15000.00	831.57
363.15	20000.00	836.11
363.15	25000.00	840.56
363.15	30000.00	845.01
363.15	35000.00	849.23
363.15	40000.00	853.33
363.15	50000.00	860.82
363.15	60000.00	867.91

Reference

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

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
294.20	107.00	0.0011100
294.13	4967.00	0.0011700
293.85	9970.00	0.0012200
293.58	14994.00	0.0012800
292.87	19994.00	0.0013500
292.56	25040.00	0.0014200
292.04	30028.00	0.0015000
303.15	102.00	0.0009500
303.12	5011.00	0.0010000
303.08	10026.00	0.0010500
303.05	14993.00	0.0011000
303.02	19985.00	0.0011500
302.93	25017.00	0.0012000
302.83	29961.00	0.0012400
312.77	103.00	0.0008300
312.78	5010.00	0.0008800
312.65	10009.00	0.0009200
312.66	15001.00	0.0009700
312.62	20047.00	0.0010100
312.57	25001.00	0.0010500
312.49	29986.00	0.0010900
322.33	96.00	0.0007300
322.26	5004.00	0.0007700
322.23	10018.00	0.0008100
322.21	15004.00	0.0008500
322.17	19955.00	0.0008900
322.23	25027.00	0.0009300
322.09	29925.00	0.0009700
331.85	99.00	0.0006500
331.78	5007.00	0.0006900
331.78	9972.00	0.0007200
331.74	15035.00	0.0007600
331.67	19865.00	0.0008000
331.68	25041.00	0.0008300
331.56	30001.00	0.0008700
341.67	96.00	0.0005800
341.72	5062.00	0.0006200
341.68	10141.00	0.0006500
341.48	14961.00	0.0006900

341.81	20048.00	0.0007200
341.80	25032.00	0.0007500
341.73	29980.00	0.0007800
351.27	10077.00	0.0005800
351.26	14966.00	0.0006100
351.31	19977.00	0.0006400
351.49	24997.00	0.0006700
351.46	30010.00	0.0007000
361.37	20002.00	0.0005800
361.47	25022.00	0.0006100
361.24	29993.00	0.0006400

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<https://www.doi.org/10.1016/j.jct.2019.02.026>

Sources

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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
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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