

# Nonanoic acid, methyl ester

<b>Other names:</b>	Methyl ester nonanoic acid Methyl ester of nonanoic acid Methyl n-nonanoate Methyl nonanoate Methyl nonylate Methyl pelargonate Pelargonic acid methyl ester pelargonic acid, methyl ester
<b>Inchi:</b>	InChI=1S/C10H20O2/c1-3-4-5-6-7-8-9-10(11)12-2/h3-9H2,1-2H3
<b>InchiKey:</b>	IJXHLVMUNBOGRR-UHFFFAOYSA-N
<b>Formula:</b>	C10H20O2
<b>SMILES:</b>	CCCCCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	172.26
<b>CAS:</b>	1731-84-6

## Physical Properties

Property code	Value	Unit	Source
chl	-6176.80 ± 1.50	kJ/mol	NIST Webbook
gf	-200.60	kJ/mol	Joback Method
hf	-494.53	kJ/mol	Joback Method
hfus	27.34	kJ/mol	Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K
hvap	47.01	kJ/mol	Joback Method
log10ws	-3.38		Aqueous Solubility Prediction Method
log10ws	-3.38		Estimated Solubility Method
logp	2.910		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1206.28		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1206.00		NIST Webbook

rinpol	1209.00	NIST Webbook
rinpol	1204.00	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1215.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1210.70	NIST Webbook
rinpol	1210.70	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1222.00	NIST Webbook
rinpol	1228.50	NIST Webbook
rinpol	1229.40	NIST Webbook
rinpol	1205.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1209.00	NIST Webbook
rinpol	1215.00	NIST Webbook
rinpol	1216.00	NIST Webbook
rinpol	1222.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1227.30	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1226.00	NIST Webbook
rinpol	1209.00	NIST Webbook
rinpol	1226.00	NIST Webbook
rinpol	1205.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1209.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1213.00	NIST Webbook
rinpol	1211.00	NIST Webbook

ripol	1213.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	211.60		NIST Webbook
ripol	205.30		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1206.38		NIST Webbook
ripol	1205.74		NIST Webbook
ripol	1205.64		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1508.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1491.00		NIST Webbook
tb	486.70 ± 2.00	K	NIST Webbook
tb	486.85 ± 0.35	K	NIST Webbook
tb	486.70	K	NIST Webbook
tc	676.79	K	Joback Method
tf	238.80 ± 0.05	K	NIST Webbook
vc	0.620	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.11	J/mol×K	504.49	Joback Method
cpg	382.26	J/mol×K	533.21	Joback Method
cpg	395.89	J/mol×K	561.92	Joback Method
cpg	409.00	J/mol×K	590.64	Joback Method
cpg	421.59	J/mol×K	619.36	Joback Method
cpg	433.67	J/mol×K	648.08	Joback Method
cpg	445.25	J/mol×K	676.79	Joback Method
cpl	351.70	J/mol×K	303.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	372.80	J/mol×K	353.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	367.90	J/mol×K	343.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	377.60	J/mol×K	363.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	382.00	J/mol×K	373.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	354.70	J/mol×K	313.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	363.10	J/mol×K	333.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters

cpl	358.60	J/mol×K	323.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
dvisc	0.0002904	Paxs	466.18	Joback Method
dvisc	0.0003964	Paxs	427.87	Joback Method
dvisc	0.0005753	Paxs	389.56	Joback Method
dvisc	0.0009057	Paxs	351.24	Joback Method
dvisc	0.0015931	Paxs	312.93	Joback Method
dvisc	0.0002230	Paxs	504.49	Joback Method
dvisc	0.0032806	Paxs	274.62	Joback Method
hvapt	55.60	kJ/mol	401.50	NIST Webbook
hvapt	57.40	kJ/mol	350.00	NIST Webbook
hvapt	56.70 ± 0.30	kJ/mol	364.00	NIST Webbook
tcondl	0.13	W/m×K	338.16	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	358.24	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	363.07	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	368.10	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.12	W/m×K	373.11	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	378.24	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.12	W/m×K	383.21	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	328.25	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	323.25	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	318.29	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	313.30	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.14	W/m×K	308.24	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	303.31	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	298.30	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	293.36	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	288.50	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	283.50	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.14	W/m×K	278.44	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel

tcondl	0.13	W/m×K	353.12	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	348.07	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	333.06	Experimental investigations on the liquid thermal conductivity of five saturated fatty acid methyl esters components of biodiesel
tcondl	0.13	W/m×K	343.23	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	1.50470e+01
Coeff. B	-4.27846e+03
Coeff. C	-7.64390e+01
Temperature range (K), min.	366.32
Temperature range (K), max.	515.91



# Datasets

## Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	100.00	874.53
293.15	1000.00	874.57
293.15	3000.00	876.13
293.15	5000.00	877.24
293.15	10000.00	880.79
293.15	15000.00	884.05
293.15	20000.00	887.23
293.15	25000.00	890.33
293.15	30000.00	893.33
293.15	35000.00	896.14
293.15	40000.00	898.87
293.15	50000.00	904.41
293.15	60000.00	909.15
303.15	100.00	865.62
303.15	1000.00	866.39
303.15	3000.00	867.88
303.15	5000.00	869.35
303.15	10000.00	872.9
303.15	15000.00	876.32
303.15	20000.00	879.53
303.15	25000.00	882.74
303.15	30000.00	885.85
303.15	35000.00	888.79
303.15	40000.00	891.61
303.15	50000.00	897.21
303.15	60000.00	902.44
313.15	100.00	857.46
313.15	1000.00	857.68
313.15	3000.00	859.33
313.15	5000.00	860.86
313.15	10000.00	864.63
313.15	15000.00	868.21
313.15	20000.00	871.68
313.15	25000.00	875.06
313.15	30000.00	878.23

313.15	35000.00	881.36
313.15	40000.00	884.18
313.15	50000.00	890.09
313.15	60000.00	895.33
323.15	100.00	848.37
323.15	1000.00	849.17
323.15	3000.00	850.82
323.15	5000.00	852.43
323.15	10000.00	856.42
323.15	15000.00	860.21
323.15	20000.00	863.98
323.15	25000.00	867.27
323.15	30000.00	870.68
323.15	35000.00	873.86
323.15	40000.00	877.04
323.15	50000.00	883.08
323.15	60000.00	888.79
333.15	100.00	839.92
333.15	1000.00	840.72
333.15	3000.00	842.6
333.15	5000.00	844.26
333.15	10000.00	848.44
333.15	15000.00	852.27
333.15	20000.00	856.18
333.15	25000.00	859.9
333.15	30000.00	863.32
333.15	35000.00	866.68
333.15	40000.00	870.12
333.15	50000.00	876.13
333.15	60000.00	881.95
343.15	100.00	831.17
343.15	1000.00	832.28
343.15	3000.00	834.1
343.15	5000.00	835.98
343.15	10000.00	840.27
343.15	15000.00	844.44
343.15	20000.00	848.65
343.15	25000.00	852.29
343.15	30000.00	856.04
343.15	35000.00	859.58
343.15	40000.00	862.91
343.15	50000.00	869.47
343.15	60000.00	875.25
353.15	100.00	822.78

353.15	1000.00	823.57
353.15	3000.00	825.7
353.15	5000.00	827.54
353.15	10000.00	832.17
353.15	15000.00	836.71
353.15	20000.00	840.79
353.15	25000.00	844.86
353.15	30000.00	848.7
353.15	35000.00	852.44
353.15	40000.00	855.87
353.15	50000.00	862.53
353.15	60000.00	868.9
363.15	100.00	814.24
363.15	1000.00	815.28
363.15	3000.00	817.47
363.15	5000.00	819.49
363.15	10000.00	824.1
363.15	15000.00	829.08
363.15	20000.00	833.26
363.15	25000.00	837.27
363.15	30000.00	841.4
363.15	35000.00	845.31
363.15	40000.00	849.11
363.15	50000.00	855.98
363.15	60000.00	862.59

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
299.19	103.00	0.0015600
298.77	4957.00	0.0016500
298.42	9955.00	0.0017300
298.08	14977.00	0.0018300
297.81	20011.00	0.0019300
297.50	24979.00	0.0020100
297.15	30034.00	0.0021100
303.10	106.00	0.0014600
303.08	4961.00	0.0015400
303.01	9972.00	0.0016200

303.09	15047.00	0.0016800
303.09	19964.00	0.0017600
302.91	24994.00	0.0018300
302.95	30000.00	0.0019100
312.38	99.00	0.0012600
312.32	4993.00	0.0013200
312.28	9996.00	0.0013800
312.28	14963.00	0.0014300
312.27	19968.00	0.0015000
312.19	25005.00	0.0015700
312.06	29961.00	0.0016500
321.64	96.00	0.0010800
321.60	4982.00	0.0011400
321.56	10020.00	0.0012000
321.61	15017.00	0.0012500
321.49	19988.00	0.0013100
321.36	24985.00	0.0013600
321.26	29949.00	0.0014200
331.26	108.00	0.0009400
331.23	5027.00	0.0009900
331.13	9979.00	0.0010400
331.20	14998.00	0.0010900
330.94	19996.00	0.0011400
331.13	25032.00	0.0011900
330.93	30013.00	0.0012400
341.21	96.00	0.0008100
341.03	4962.00	0.0008600
341.06	10010.00	0.0009100
341.14	15019.00	0.0009400
340.91	19959.00	0.0009900
340.95	25015.00	0.0010400
340.96	30009.00	0.0010800
351.04	101.00	0.0007100
350.95	4985.00	0.0007500
350.88	9984.00	0.0007900
350.81	14959.00	0.0008300
350.86	20020.00	0.0008700
350.74	24964.00	0.0009200
350.73	29961.00	0.0009600
360.96	98.00	0.0006200
360.86	4959.00	0.0006600
360.82	9960.00	0.0007000
360.89	14997.00	0.0007400
360.71	19982.00	0.0007700

360.61	25005.00	0.0008200
360.67	29996.00	0.0008500

Reference

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

## Sources

High-pressure liquid densities of fatty acid methyl esters: Measurement and Prediction with the Peng-Robinson equation of state	<a href="https://www.doi.org/10.1016/j.fluid.2018.04.024">https://www.doi.org/10.1016/j.fluid.2018.04.024</a>
Experimental investigation on the liquid thermal conductivity of five saturated fatty acid methyl esters	<a href="https://www.doi.org/10.1016/j.jct.2018.05.019">https://www.doi.org/10.1016/j.jct.2018.05.019</a>
Aqueous Solubility Prediction Method: components of biodiesel	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters	<a href="https://www.doi.org/10.1016/j.jct.2018.09.024">https://www.doi.org/10.1016/j.jct.2018.09.024</a>
McGowan Method:	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
Liquid viscosities for methyl hexanoate, methyl heptanoate, methyl octanoate, methyl nonanoate and methyl decanoate	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
The Yaws Handbook of Vapor Pressure: Critical Pressures:	<a href="https://www.doi.org/10.1016/j.jct.2019.02.026">https://www.doi.org/10.1016/j.jct.2019.02.026</a>
NIST Webbook:	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
Crippen Method:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731846&amp;Units=SI</a>
Joback Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methylleicosanoate between 5 K and 350 K:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
	<a href="https://www.doi.org/10.1021/je0499364">https://www.doi.org/10.1021/je0499364</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices

<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tcondl:</b>	Liquid thermal conductivity
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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