

Heptanoic acid, ethyl ester

Other names:	AETHER OENANTHICUS
	Cognac oil
	ENANTHYLIC ETHER
	ETHYL HEPTANOATE
	Enanthic acid ethyl ester
	Ethyl enanthate
	Ethyl ester of heptanoic acid
	Ethyl heptoate
	Ethyl heptylate
	Ethyl n-heptanoate
	Ethyl oenanthate
	Ethyl oenanthylate
	Grape oil
	NSC 8891
	Oenanthic ether
	Oleum vitis viniferae
	Wine oil
	ethyl enantate
Inchi:	InChI=1S/C9H18O2/c1-3-5-6-7-8-9(10)11-4-2/h3-8H2,1-2H3
InchiKey:	TVQGDYNRXLTQAP-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCC(=O)OCC
Mol. weight [g/mol]:	158.24
CAS:	106-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-548.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-603.80 ± 1.50	kJ/mol	NIST Webbook
hfus	21.85	kJ/mol	Joback Method
hvap	56.00 ± 1.00	kJ/mol	NIST Webbook
hvap	55.80	kJ/mol	NIST Webbook
log10ws	-2.71		Aqueous Solubility Prediction Method
log10ws	-2.74		Estimated Solubility Method

logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2356.90	kPa	Development of a Predictive Equation of State for CO ₂ + Ethyl Ester Mixtures Based on Critical Points Measurements
rinpol	1097.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1093.30		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1098.00		NIST Webbook
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rinpol	1085.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1093.30		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1108.00		NIST Webbook

rinpol	1099.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1068.00	NIST Webbook
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rinpol	1082.00	NIST Webbook
rinpol	1093.00	NIST Webbook
ripol	1334.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1345.00	NIST Webbook
ripol	1331.00	NIST Webbook
ripol	1336.00	NIST Webbook
ripol	1332.00	NIST Webbook
ripol	1325.00	NIST Webbook
ripol	1336.00	NIST Webbook
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ripol	1375.00	NIST Webbook
ripol	1325.00	NIST Webbook
ripol	1369.00	NIST Webbook
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ripol	1332.00	NIST Webbook

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ripol	1329.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	461.70	K	NIST Webbook
tb	461.70 ± 0.30	K	NIST Webbook
tb	460.30 ± 2.00	K	NIST Webbook

tb	461.70	K	KDB
tc	634.30 ± 0.60	K	NIST Webbook
tf	207.12	K	Aqueous Solubility Prediction Method
tf	207.05	K	KDB
tf	206.90 ± 0.50	K	NIST Webbook
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/mol×K	481.61	Joback Method
cpg	336.15	J/mol×K	510.56	Joback Method
cpg	348.92	J/mol×K	539.50	Joback Method
cpg	361.21	J/mol×K	568.45	Joback Method
cpg	373.04	J/mol×K	597.40	Joback Method
cpg	384.40	J/mol×K	626.35	Joback Method
cpg	395.29	J/mol×K	655.29	Joback Method
dvisc	0.0033103	Pa×s	263.35	Joback Method
dvisc	0.0016384	Pa×s	299.73	Joback Method
dvisc	0.0009442	Pa×s	336.10	Joback Method
dvisc	0.0006060	Pa×s	372.48	Joback Method
dvisc	0.0004209	Pa×s	408.86	Joback Method
dvisc	0.0003103	Pa×s	445.23	Joback Method
dvisc	0.0002395	Pa×s	481.61	Joback Method
rfi	1.38421		358.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41784		283.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41562		288.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41341		293.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.41119		298.15	Thermophysical properties of fatty acid methyl and ethyl esters

rfi	1.40896		303.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40673		308.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40445		313.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.40216		318.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39988		323.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.42006		278.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39535		333.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39311		338.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39088		343.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38866		348.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.38645		353.15	Thermophysical properties of fatty acid methyl and ethyl esters
rfi	1.39761		328.15	Thermophysical properties of fatty acid methyl and ethyl esters
rhoI	881.30	kg/m3	293.15	Phase equilibrium of (water + formic or acetic acid + ethyl heptanoate) ternary liquid systems at different temperatures

tcondl	0.13	W/m×K	329.73	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.15	W/m×K	260.21	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.14	W/m×K	270.16	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.14	W/m×K	280.02	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.14	W/m×K	289.93	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.14	W/m×K	299.84	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.13	W/m×K	309.90	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel

tcondl	0.13	W/m×K	319.73	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	
tcondl	0.15	W/m×K	250.38	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	
tcondl	0.13	W/m×K	337.72	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	
tcondl	0.13	W/m×K	341.71	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	
tcondl	0.13	W/m×K	347.65	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	
tcondl	0.12	W/m×K	353.60	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	
tcondl	0.12	W/m×K	363.50	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel	

tcondl	0.12	W/m×K	373.51	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.12	W/m×K	383.64	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel
tcondl	0.11	W/m×K	393.46	Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53528e+01
Coeff. B	-4.15873e+03
Coeff. C	-6.90720e+01
Temperature range (K), min.	345.12
Temperature range (K), max.	483.23

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
303.20	100.00	860.8
303.20	3020.00	864.5
303.10	6000.00	867.7
303.20	9010.00	871.2
303.21	11950.00	874.5
303.19	14980.00	877.5
312.96	100.00	851.2
313.06	3060.00	854.7
313.13	6090.00	858.1
313.17	9070.00	861.4
313.18	12000.00	864.7
313.17	15010.00	867.9
323.09	100.00	841.6
323.11	3100.00	845.2
323.14	6110.00	848.8
323.10	9100.00	852.5
323.13	12060.00	855.8
323.09	15150.00	859.2
333.05	100.00	832.1
333.14	3010.00	835.6
333.18	6080.00	839.7
333.14	9020.00	843.2
333.14	12010.00	846.8
333.20	15070.00	850.5
343.02	100.00	823.0
343.06	3010.00	827.1
343.23	6050.00	831.0
343.20	9000.00	834.8
343.22	12100.00	838.5
343.19	15000.00	842.1
352.85	100.00	815.1
352.95	3090.00	819.4
353.11	6070.00	823.2
353.06	9090.00	827.5
353.14	12070.00	831.2

353.23	15010.00	835.1
Reference		https://www.doi.org/10.1021/acs.jced.7b00386

Speed of sound, m/s

Temperature, K - Liquid	Pressure, kPa - Liquid	Speed of sound, m/s - Liquid
293.27	110.00	1254.03
303.20	100.00	1219.89
313.04	90.00	1185.84
323.08	110.00	1145.28
332.61	100.00	1119.94
343.14	100.00	1075.42
353.04	110.00	1044.19
363.11	100.00	1008.42
372.84	90.00	971.9
382.87	100.00	941.96
392.49	100.00	909.29
401.72	110.00	876.2
412.92	100.00	837.29
422.78	110.00	800.01
432.75	100.00	768.89
441.74	90.00	736.98
452.13	100.00	703.21
293.55	1040.00	1263.87
302.87	1020.00	1230.26
313.07	1000.00	1189.64
323.15	1020.00	1154.57
332.75	980.00	1123.74
343.15	1020.00	1086.84
352.67	1000.00	1053.08
362.35	1010.00	1014.12
371.83	1020.00	987.06
382.34	1020.00	948.49
392.73	980.00	912.95
401.77	1030.00	883.74
412.69	1050.00	841.82
422.42	1000.00	807.44
432.36	1120.00	778.68
441.56	1020.00	750.38
451.89	990.00	714.64

462.89	1110.00	677.9
471.98	1010.00	647.85
482.54	1000.00	610.64
293.40	2560.00	1278.44
303.46	2500.00	1233.57
313.11	2510.00	1200.03
323.11	2490.00	1164.66
332.84	2500.00	1127.35
451.94	2540.00	731.06
463.03	2520.00	699.91
472.16	2540.00	667.91
482.35	2490.00	636.04
293.20	4000.00	1290.82
303.00	4050.00	1253.21
312.99	4070.00	1207.7
323.12	3990.00	1173.82
332.85	4010.00	1140.43
343.20	4050.00	1101.44
352.64	4010.00	1073.47
362.37	4060.00	1038.84
371.97	4040.00	1005.36
382.36	3940.00	970.18
392.65	4020.00	936.25
401.75	4030.00	907.66
412.64	4050.00	868.48
422.45	4040.00	836.46
432.43	4070.00	805.62
441.62	4050.00	783.09
452.05	4040.00	748.01
463.13	4040.00	714.4
472.23	4040.00	687.28
483.02	4020.00	655.14
293.74	5550.00	1291.01
303.04	5540.00	1254.0
313.12	5550.00	1223.42
323.12	5530.00	1181.98
333.57	5530.00	1140.54
343.18	5510.00	1114.79
352.70	5540.00	1079.0
362.26	5530.00	1045.42
372.00	5590.00	1016.18
382.32	5500.00	983.52
392.67	5520.00	946.64
401.62	5620.00	919.87

412.54	5550.00	885.03
422.48	5560.00	854.66
432.45	5500.00	819.99
441.62	5570.00	795.09
452.08	5580.00	763.54
463.22	5530.00	728.32
382.36	7030.00	991.78
392.69	6990.00	960.26
401.59	6980.00	932.15
412.71	7010.00	898.63
422.53	6970.00	866.85
432.47	6990.00	831.89
441.61	7020.00	810.86
452.07	7050.00	781.2
463.25	7020.00	748.5
472.22	7040.00	716.46
483.13	7020.00	690.38
294.07	8560.00	1302.85
303.06	8580.00	1271.63
313.03	8520.00	1229.84
323.14	8520.00	1198.91
332.87	8520.00	1168.42
343.18	8540.00	1133.1
352.86	8580.00	1098.06
362.06	8560.00	1073.66
372.00	8580.00	1035.47
382.40	8550.00	1003.61
392.72	8520.00	974.33
401.43	8550.00	945.5
412.77	8460.00	910.68
422.49	8460.00	880.79
432.50	8520.00	845.66
441.61	8500.00	822.18
452.07	8500.00	791.7
463.26	8550.00	758.92
472.22	8560.00	727.9
483.34	8540.00	700.94
293.99	10050.00	1302.01
303.06	10060.00	1275.7
313.06	9950.00	1235.73
323.14	9970.00	1202.86
332.88	10020.00	1171.25
343.18	10030.00	1146.59
352.81	9950.00	1114.93

362.02	9960.00	1086.09
372.00	9980.00	1054.29
382.38	10030.00	1013.95
392.70	10020.00	988.42
342.92	2540.00	1095.65
352.61	2510.00	1056.91
362.38	2500.00	1028.17
371.91	2580.00	995.52
382.38	2510.00	958.12
392.65	2490.00	924.2
401.70	2510.00	892.06
412.73	2540.00	858.95
422.35	2540.00	826.98
432.43	2500.00	790.22
441.59	2560.00	766.2
472.22	5550.00	706.95
483.07	5540.00	677.03
293.91	7040.00	1299.58
303.06	7040.00	1262.89
313.09	7070.00	1225.84
323.13	7000.00	1188.04
332.88	7010.00	1156.97
343.18	7060.00	1119.21
352.76	7070.00	1088.79
361.99	7040.00	1061.57
372.00	7060.00	1029.84
401.51	10090.00	955.49
412.74	10010.00	920.21
422.51	9930.00	896.93
432.49	10010.00	865.32
441.61	10030.00	837.4
452.07	10040.00	804.8
463.25	10030.00	765.58
472.22	10050.00	743.93
483.14	10030.00	706.31

Reference

<https://www.doi.org/10.1016/j.fluid.2016.10.006>

Molar heat capacity at constant pressure, J/K/mol

Temperature, K - Liquid

Pressure, kPa - Liquid

Molar heat capacity at constant
pressure, J/K/mol - Liquid

305.40	100.00	318.30
305.40	4040.00	317.70
305.40	8190.00	317.30
305.40	12090.00	316.80
305.50	16070.00	316.40
315.70	100.00	322.50
315.80	4190.00	322.00
315.90	8150.00	321.60
315.90	12260.00	320.50
316.00	16160.00	319.60
326.50	100.00	326.80
326.50	4140.00	325.90
326.60	8170.00	325.20
326.60	12110.00	324.30
326.20	16030.00	323.60
335.30	100.00	330.30
335.30	4060.00	330.10
335.40	8050.00	328.60
335.40	12030.00	327.60
335.50	16070.00	326.90
345.10	100.00	334.20
345.20	4070.00	333.50
345.60	8230.00	332.50
345.70	12160.00	332.20
345.70	16230.00	330.50
354.20	100.00	337.80
354.20	4120.00	337.30
354.30	8010.00	336.50
354.40	12390.00	335.60
354.50	16250.00	334.50
364.90	100.00	342.10
365.30	3870.00	341.30
365.60	8320.00	340.30
365.70	12160.00	339.50
365.80	15950.00	338.30
374.80	100.00	346.10
375.00	3980.00	345.50
375.50	8020.00	344.00
375.70	12070.00	342.60
375.90	16040.00	341.40
384.00	100.00	349.80
385.00	4020.00	349.10
385.40	8040.00	347.10
385.50	11880.00	346.10

385.70	15890.00	345.60
Reference		https://www.doi.org/10.1016/j.jct.2015.09.031

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.chemic.org/files/research/kdb/mol/mol1111.mol
Measurement of speed of sound and thermal diffusivity of ethyl heptanoate	https://www.doi.org/10.1016/j.fluid.2016.10.006
Binary Equilibrium (Method: formic or acetic acid + ethyl heptanoate) ternary liquid system at different temperatures:	https://www.doi.org/10.1016/j.fluid.2013.07.015
The Yaws Handbook of Vapor Pressure:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities and Viscosities of Ethyl Heptanoate and Ethyl Octanoate at	http://link.springer.com/article/10.1007/BF02311772
Thermophysical Properties of Ethyl Heptanoate and Ethyl Octanoate	https://www.doi.org/10.1021/acs.jced.7b00386
Isobaric heat capacities of ethyl heptanoate and ethyl cinnamate at	https://www.doi.org/10.1016/j.jct.2019.02.025
Measurement of a 3-Parameter Equation of State for CO ₂ + Ethyl Ester Mixtures	https://www.doi.org/10.1016/j.jct.2015.09.031
NIST Webbook	https://www.doi.org/10.1021/je5002494
Measurements:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106309&Units=SI
Measurement on the thermal conductivity of five saturated fatty acid	https://www.doi.org/10.1016/j.fluid.2018.06.004
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

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
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
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume

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