

methyl 2-hydroxypropanoate

Other names:	(.+-)-methyl 2-hydroxypropanoate (.+-)-methyl 2-hydroxypropionate (.+-)-methyl lactate 2-hydroxypropanoic acid methyl ester Propanoic acid, 2-hydroxy, methyl ester lactic acid methyl ester lactic acid, methyl ester methyl .alpha.-hydroxypropionate methyl 2-hydroxypropionate methyl lactate propanoic acid, 2-hydroxy-, methyl ester
Inchi:	InChI=1S/C4H8O3/c1-3(5)4(6)7-2/h3,5H,1-2H3
InchiKey:	LPEKGGXMPWTOCB-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	COC(=O)C(C)O
Mol. weight [g/mol]:	104.10
CAS:	547-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-390.38	kJ/mol	Joback Method
hf	-528.20	kJ/mol	Joback Method
hfus	9.47	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	0.27		Crippen Method
logp	-0.460		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	417.00 ± 0.50	K	NIST Webbook
tb	417.00 ± 0.50	K	NIST Webbook
tb	417.00 ± 0.50	K	NIST Webbook
tc	636.26	K	Joback Method
tf	252.82	K	Joback Method
vc	0.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.54	J/molxK	547.60	Joback Method
cpg	172.74	J/molxK	488.50	Joback Method
cpg	179.25	J/molxK	518.05	Joback Method
cpg	191.62	J/molxK	577.16	Joback Method
cpg	197.46	J/molxK	606.71	Joback Method
cpg	203.08	J/molxK	636.26	Joback Method
cpg	166.01	J/molxK	458.95	Joback Method
dvisc	0.0012346	Paxs	355.88	Joback Method
dvisc	0.0028726	Paxs	321.53	Joback Method
dvisc	0.0006157	Paxs	390.24	Joback Method
dvisc	0.0309613	Paxs	252.82	Joback Method
dvisc	0.0081807	Paxs	287.18	Joback Method
dvisc	0.0003436	Paxs	424.59	Joback Method
dvisc	0.0002093	Paxs	458.95	Joback Method
hvapt	44.70	kJ/mol	365.50	NIST Webbook
pvap	0.87	kPa	303.15	Isothermal Vapor-Liquid Equilibrium, Excess Enthalpy Data and Activity Coefficients at Infinite Dilution for the Binary System Water + Methyl Lactate
pvap	0.43	kPa	293.15	Isothermal Vapor-Liquid Equilibrium, Excess Enthalpy Data and Activity Coefficients at Infinite Dilution for the Binary System Water + Methyl Lactate
pvap	0.17	kPa	283.15	Isothermal Vapor-Liquid Equilibrium, Excess Enthalpy Data and Activity Coefficients at Infinite Dilution for the Binary System Water + Methyl Lactate
rho1	1062.01	kg/m3	320.65	Thermophysical Properties of Lactates

rhoI	1070.55	kg/m3	313.15	Thermophysical Properties of Lactates
rhoI	1067.71	kg/m3	315.65	Thermophysical Properties of Lactates
rhoI	1064.86	kg/m3	318.15	Thermophysical Properties of Lactates
rhoI	1073.38	kg/m3	310.65	Thermophysical Properties of Lactates
rhoI	1059.15	kg/m3	323.15	Thermophysical Properties of Lactates
rhoI	1056.28	kg/m3	325.65	Thermophysical Properties of Lactates
rhoI	1053.40	kg/m3	328.15	Thermophysical Properties of Lactates
rhoI	1050.52	kg/m3	330.65	Thermophysical Properties of Lactates
rhoI	1047.63	kg/m3	333.15	Thermophysical Properties of Lactates
rhoI	1044.73	kg/m3	335.65	Thermophysical Properties of Lactates
rhoI	1041.83	kg/m3	338.15	Thermophysical Properties of Lactates
rhoI	1076.20	kg/m3	308.15	Thermophysical Properties of Lactates
rhoI	1079.02	kg/m3	305.65	Thermophysical Properties of Lactates
rhoI	1081.83	kg/m3	303.15	Thermophysical Properties of Lactates
rhoI	1084.64	kg/m3	300.65	Thermophysical Properties of Lactates
rhoI	1087.43	kg/m3	298.15	Thermophysical Properties of Lactates
rhoI	1090.23	kg/m3	295.65	Thermophysical Properties of Lactates
rhoI	1093.01	kg/m3	293.15	Thermophysical Properties of Lactates
rhoI	1095.79	kg/m3	290.65	Thermophysical Properties of Lactates

rhoI	1098.57	kg/m3	288.15	Thermophysical Properties of Lactates
rhoI	1101.34	kg/m3	285.65	Thermophysical Properties of Lactates
rhoI	1104.11	kg/m3	283.15	Thermophysical Properties of Lactates
rhoI	1106.86	kg/m3	280.65	Thermophysical Properties of Lactates
rhoI	1087.43	kg/m3	298.15	Self-aggregation of liquids from biomass in aqueous solution
rhoI	1109.61	kg/m3	278.15	Thermophysical Properties of Lactates

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	1104.41
288.15	100.00	1098.86
293.15	100.00	1093.31
298.15	100.00	1087.76
303.15	100.00	1082.13
308.15	100.00	1076.53
313.15	100.00	1070.85
318.15	100.00	1065.11
323.15	100.00	1059.39
328.15	100.00	1053.63
333.15	100.00	1047.83
338.15	100.00	1042.0
283.15	2500.00	1106.0
288.15	2500.00	1100.48
293.15	2500.00	1094.99
298.15	2500.00	1089.42
303.15	2500.00	1083.92
308.15	2500.00	1078.32

313.15	2500.00	1072.76
318.15	2500.00	1067.04
323.15	2500.00	1061.4
328.15	2500.00	1055.7
333.15	2500.00	1049.97
338.15	2500.00	1044.15
283.15	5000.00	1107.57
288.15	5000.00	1102.13
293.15	5000.00	1096.72
298.15	5000.00	1091.21
303.15	5000.00	1085.75
308.15	5000.00	1080.19
313.15	5000.00	1074.65
318.15	5000.00	1068.97
323.15	5000.00	1063.43
328.15	5000.00	1057.77
333.15	5000.00	1052.16
338.15	5000.00	1046.35
283.15	7500.00	1109.14
288.15	7500.00	1103.77
293.15	7500.00	1098.35
298.15	7500.00	1092.88
303.15	7500.00	1087.5
308.15	7500.00	1082.0
313.15	7500.00	1076.52
318.15	7500.00	1070.94
323.15	7500.00	1065.44
328.15	7500.00	1059.74
333.15	7500.00	1054.23
338.15	7500.00	1048.52
283.15	10000.00	1110.68
288.15	10000.00	1105.31
293.15	10000.00	1099.92
298.15	10000.00	1094.57
303.15	10000.00	1089.23
308.15	10000.00	1083.79
313.15	10000.00	1078.39
318.15	10000.00	1072.77
323.15	10000.00	1067.34
328.15	10000.00	1061.8
333.15	10000.00	1056.23
338.15	10000.00	1050.63
283.15	20000.00	1116.59
288.15	20000.00	1111.55

293.15	20000.00	1106.2
298.15	20000.00	1101.03
303.15	20000.00	1095.82
308.15	20000.00	1090.68
313.15	20000.00	1085.28
318.15	20000.00	1080.09
323.15	20000.00	1074.67
328.15	20000.00	1069.41
333.15	20000.00	1064.05
338.15	20000.00	1058.63
283.15	30000.00	1122.23
288.15	30000.00	1117.27
293.15	30000.00	1112.08
298.15	30000.00	1107.23
303.15	30000.00	1101.97
308.15	30000.00	1097.03
313.15	30000.00	1091.84
318.15	30000.00	1086.77
323.15	30000.00	1081.41
328.15	30000.00	1076.5
333.15	30000.00	1071.33
338.15	30000.00	1066.13
283.15	40000.00	1127.45
288.15	40000.00	1122.78
293.15	40000.00	1117.65
298.15	40000.00	1112.83
303.15	40000.00	1107.9
308.15	40000.00	1102.99
313.15	40000.00	1097.99
318.15	40000.00	1093.08
323.15	40000.00	1088.0
328.15	40000.00	1083.15
333.15	40000.00	1078.01
338.15	40000.00	1073.12
283.15	50000.00	1132.48
288.15	50000.00	1127.98
293.15	50000.00	1122.93
298.15	50000.00	1118.24
303.15	50000.00	1113.44
308.15	50000.00	1108.63
313.15	50000.00	1103.74
318.15	50000.00	1098.93
323.15	50000.00	1094.04
328.15	50000.00	1089.4

333.15	50000.00	1084.39
338.15	50000.00	1079.74
283.15	60000.00	1137.4
288.15	60000.00	1132.78
293.15	60000.00	1128.01
298.15	60000.00	1123.43
303.15	60000.00	1118.66
308.15	60000.00	1114.02
313.15	60000.00	1109.24
318.15	60000.00	1104.49
323.15	60000.00	1099.76
328.15	60000.00	1095.07
333.15	60000.00	1090.37
338.15	60000.00	1085.76

Reference

<https://www.doi.org/10.1016/j.jct.2012.11.002>

Temperature, K	Pressure, kPa	Mass density, kg/m3
298.15	100.00	1087.35

Reference

<https://www.doi.org/10.1016/j.jct.2018.07.013>

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C547648&Units=SI>

The pqT behaviour of the lactate family: <https://www.doi.org/10.1016/j.jct.2012.11.002>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Thermodynamic behaviour of alkyl lactate-alkanol systems: <https://www.doi.org/10.1016/j.jct.2018.07.013>

Thermophysical Properties of Lactates: <https://www.doi.org/10.1016/j.tca.2013.11.010>

Isothermal Vapor-Liquid Equilibrium, Excess Enthalpy Data and Activity Coefficients at Infinite Dilution for the Binary System Water + Methyl Lactate: <https://www.doi.org/10.1021/je049824c>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Self-aggregation of liquids from biomass in aqueous solution: <https://www.doi.org/10.1016/j.jct.2013.06.020>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

High-Pressure Phase Behavior of Methyl Lactate and Ethyl Lactate in Supercritical Carbon Dioxide: <https://www.doi.org/10.1021/je200299s>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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