

2-Furancarboxaldehyde, 5-methyl-

Other names:	2-Formyl-5-methylfuran 2-Furaldehyde, 5-methyl- 2-Methyl-5-formylfuran 5-Methylfurfural 5-Methyl-2-furaldehyde 5-Methyl-2-furanaldehyde 5-Methyl-2-furancarbaldehyde 5-Methyl-2-furancarboxaldehyde 5-Methyl-2-furancarboxaldehyde (5-methylfurfural) 5-Methyl-2-furancarboxyaldehyde 5-Methyl-2-furfural 5-Methyl-2-furfuraldehyde 5-Methylfuran-2-al 5-Methylfuran-2-carbaldehyde 5-Methylfurfuraldehyde 5-ethyl-2-furfural 5-methylfurfural Methyl-5-furfural furfural, 5-methyl-
Inchi:	InChI=1S/C6H6O2/c1-5-2-3-6(4-7)8-5/h2-4H,1H3
InchiKey:	OUDFNZMQXZILJD-UHFFFAOYSA-N
Formula:	C6H6O2
SMILES:	Cc1ccc(C=O)o1
Mol. weight [g/mol]:	110.11
CAS:	620-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.401		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
rinpol	963.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	984.00		NIST Webbook

rinpol	987.00	NIST Webbook
rinpol	941.00	NIST Webbook
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rinpol	963.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	961.00	NIST Webbook
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rinpol	980.00	NIST Webbook
rinpol	990.00	NIST Webbook
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rinpol	969.00	NIST Webbook
rinpol	980.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	958.00	NIST Webbook
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ripol	1562.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1588.00		NIST Webbook
tb	460.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	78.69	kPa	450.19	Separation of Furfural from Ternary Mixtures
pvap	0.86	kPa	339.05	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	1.13	kPa	343.25	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	1.41	kPa	347.05	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	2.00	kPa	353.15	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	2.50	kPa	357.45	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	3.00	kPa	360.95	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	4.02	kPa	366.75	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	4.52	kPa	369.25	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	6.02	kPa	376.65	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	7.02	kPa	380.15	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	8.03	kPa	383.25	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	9.04	kPa	385.95	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	10.04	kPa	388.45	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	15.02	kPa	398.25	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	19.96	kPa	405.85	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	29.89	kPa	417.55	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	3.60	kPa	365.09	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	5.18	kPa	372.92	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	3.00	kPa	359.95	Separation of Furfural from Ternary Mixtures
pvap	3.49	kPa	363.45	Separation of Furfural from Ternary Mixtures
pvap	3.99	kPa	365.85	Separation of Furfural from Ternary Mixtures
pvap	5.00	kPa	370.63	Separation of Furfural from Ternary Mixtures
pvap	4.98	kPa	370.70	Separation of Furfural from Ternary Mixtures
pvap	5.85	kPa	374.39	Separation of Furfural from Ternary Mixtures
pvap	5.99	kPa	374.75	Separation of Furfural from Ternary Mixtures
pvap	6.49	kPa	376.55	Separation of Furfural from Ternary Mixtures
pvap	29.68	kPa	415.90	Separation of Furfural from Ternary Mixtures
pvap	36.73	kPa	422.86	Separation of Furfural from Ternary Mixtures
pvap	49.52	kPa	433.44	Separation of Furfural from Ternary Mixtures
rho1	1103.20	kg/m3	298.15	Self-aggregation of liquids from biomass in aqueous solution

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	1.60	NIST Webbook

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
283.15	100.00	1118.02
288.15	100.00	1113.09
293.15	100.00	1108.15
298.15	100.00	1103.2
303.15	100.00	1098.25
308.15	100.00	1093.29
313.15	100.00	1088.32
318.15	100.00	1083.33
323.15	100.00	1078.33
328.15	100.00	1073.32
333.15	100.00	1068.3
338.15	100.00	1063.25
283.15	2500.00	1119.83
288.15	2500.00	1114.82
293.15	2500.00	1110.03
298.15	2500.00	1104.82
303.15	2500.00	1100.71
308.15	2500.00	1095.01
313.15	2500.00	1090.31
318.15	2500.00	1085.42
323.15	2500.00	1080.39
328.15	2500.00	1075.43
333.15	2500.00	1070.05
338.15	2500.00	1065.43
283.15	5000.00	1121.37

288.15	5000.00	1116.39
293.15	5000.00	1111.5
298.15	5000.00	1106.62
303.15	5000.00	1101.81
308.15	5000.00	1096.9
313.15	5000.00	1092.06
318.15	5000.00	1087.05
323.15	5000.00	1082.17
328.15	5000.00	1077.24
333.15	5000.00	1072.29
338.15	5000.00	1067.33
283.15	7500.00	1122.65
288.15	7500.00	1117.87
293.15	7500.00	1112.96
298.15	7500.00	1108.34
303.15	7500.00	1103.11
308.15	7500.00	1098.15
313.15	7500.00	1093.64
318.15	7500.00	1088.71
323.15	7500.00	1083.95
328.15	7500.00	1079.03
333.15	7500.00	1074.1
338.15	7500.00	1069.06
283.15	10000.00	1124.02
288.15	10000.00	1119.23
293.15	10000.00	1114.4
298.15	10000.00	1109.63
303.15	10000.00	1104.89
308.15	10000.00	1100.06
313.15	10000.00	1095.27
318.15	10000.00	1090.41
323.15	10000.00	1085.56
328.15	10000.00	1080.7
333.15	10000.00	1075.84
338.15	10000.00	1070.99
283.15	20000.00	1129.41
288.15	20000.00	1124.75
293.15	20000.00	1120.15
298.15	20000.00	1115.43
303.15	20000.00	1110.81
308.15	20000.00	1106.17
313.15	20000.00	1101.5
318.15	20000.00	1096.72
323.15	20000.00	1092.07

328.15	20000.00	1087.38
333.15	20000.00	1082.66
338.15	20000.00	1077.96
283.15	30000.00	1134.53
288.15	30000.00	1129.99
293.15	30000.00	1125.46
298.15	30000.00	1120.97
303.15	30000.00	1116.44
308.15	30000.00	1111.86
313.15	30000.00	1107.37
318.15	30000.00	1102.74
323.15	30000.00	1098.22
328.15	30000.00	1093.64
333.15	30000.00	1089.1
338.15	30000.00	1084.52
283.15	40000.00	1139.44
288.15	40000.00	1134.99
293.15	40000.00	1130.57
298.15	40000.00	1126.15
303.15	40000.00	1121.72
308.15	40000.00	1117.24
313.15	40000.00	1112.86
318.15	40000.00	1108.39
323.15	40000.00	1104.01
328.15	40000.00	1099.55
333.15	40000.00	1095.12
338.15	40000.00	1090.69
283.15	50000.00	1144.14
288.15	50000.00	1139.79
293.15	50000.00	1135.4
298.15	50000.00	1131.12
303.15	50000.00	1126.87
308.15	50000.00	1122.38
313.15	50000.00	1118.1
318.15	50000.00	1113.73
323.15	50000.00	1109.47
328.15	50000.00	1105.14
333.15	50000.00	1100.86
338.15	50000.00	1096.51
283.15	60000.00	1148.58
288.15	60000.00	1144.31
293.15	60000.00	1140.08
298.15	60000.00	1135.84
303.15	60000.00	1131.66

308.15	60000.00	1127.34
313.15	60000.00	1123.12
318.15	60000.00	1118.89
323.15	60000.00	1114.68
328.15	60000.00	1110.48
333.15	60000.00	1106.23
338.15	60000.00	1102.02

Reference

<https://www.doi.org/10.1021/je400783h>

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Self-aggregation of liquids from biomass in aqueous solution:	https://www.doi.org/10.1016/j.jct.2013.06.020
Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, Acetyluranyl and Methylfurfural at 3.60 and 5.18 kPa:	https://www.doi.org/10.1021/acs.jced.7b00574
Thermophysical Properties of Furfural Compounds:	https://www.doi.org/10.1021/je020117y
McGowan Method:	https://www.doi.org/10.1021/je400783h
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620020&Units=SI
	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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