

Furan, 2-ethyl-

Other names:	2-Ethylfuran 2-Ethylfurane Furan, «alpha»-ethyl- Furan, Â«alphaÂ»-ethyl-
Inchi:	InChI=1S/C6H8O/c1-2-6-4-3-5-7-6/h3-5H,2H2,1H3
InchiKey:	HLPIHRDZBHXTFJ-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	CCc1ccco1
Mol. weight [g/mol]:	96.13
CAS:	3208-16-0

Physical Properties

Property code	Value	Unit	Source
ie	8.45 ± 0.05	eV	NIST Webbook
log10ws	-6.01		Crippen Method
logp	1.842		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	702.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	730.00		NIST Webbook
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rinpol	704.00		NIST Webbook
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rinpol	707.00		NIST Webbook
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rinpol	676.00		NIST Webbook
rinpol	702.00		NIST Webbook

rinpol	689.80	NIST Webbook
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rinpol	694.00	NIST Webbook
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ripol	963.00		NIST Webbook
ripol	936.00		NIST Webbook
ripol	944.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	946.00		NIST Webbook
tb	364.40 ± 1.00	K	NIST Webbook
tb	366.65 ± 2.00	K	NIST Webbook
tb	365.25 ± 1.50	K	NIST Webbook
tb	365.15 ± 2.00	K	NIST Webbook
tb	365.65 ± 2.00	K	NIST Webbook
tb	364.00 ± 3.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	102.00	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49787e+01
Coeff. B	-3.33810e+03
Coeff. C	-4.28010e+01
Temperature range (K), min.	270.02
Temperature range (K), max.	388.10

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
283.15	100.00	915.5
288.15	100.00	910.08
293.15	100.00	904.65
298.15	100.00	899.11
303.15	100.00	893.58
308.15	100.00	888.06
313.15	100.00	882.49
318.15	100.00	876.88
323.15	100.00	871.23
328.15	100.00	865.59
333.15	100.00	859.9
338.15	100.00	854.07
283.15	2000.00	917.27
288.15	2000.00	911.89
293.15	2000.00	906.44
298.15	2000.00	901.01
303.15	2000.00	895.61
308.15	2000.00	890.15
313.15	2000.00	884.62
318.15	2000.00	879.13
323.15	2000.00	873.56
328.15	2000.00	867.92
333.15	2000.00	862.3
338.15	2000.00	856.63
283.15	5000.00	919.69
288.15	5000.00	914.37

293.15	5000.00	909.05
298.15	5000.00	903.73
303.15	5000.00	898.41
308.15	5000.00	893.04
313.15	5000.00	887.63
318.15	5000.00	882.2
323.15	5000.00	876.77
328.15	5000.00	871.27
333.15	5000.00	865.81
338.15	5000.00	860.21
283.15	7000.00	921.41
288.15	7000.00	916.19
293.15	7000.00	910.93
298.15	7000.00	905.65
303.15	7000.00	900.35
308.15	7000.00	895.02
313.15	7000.00	889.75
318.15	7000.00	884.37
323.15	7000.00	878.96
328.15	7000.00	873.57
333.15	7000.00	868.2
338.15	7000.00	862.69
283.15	10000.00	923.87
288.15	10000.00	918.68
293.15	10000.00	913.5
298.15	10000.00	908.34
303.15	10000.00	903.06
308.15	10000.00	897.93
313.15	10000.00	892.61
318.15	10000.00	887.44
323.15	10000.00	882.17
328.15	10000.00	876.84
333.15	10000.00	871.58
338.15	10000.00	866.19
283.15	15000.00	927.84
288.15	15000.00	922.7
293.15	15000.00	917.66
298.15	15000.00	912.57
303.15	15000.00	907.56
308.15	15000.00	902.45
313.15	15000.00	897.4
318.15	15000.00	892.29
323.15	15000.00	887.15
328.15	15000.00	882.03

333.15	15000.00	876.87
338.15	15000.00	871.73
283.15	20000.00	931.59
288.15	20000.00	926.63
293.15	20000.00	921.69
298.15	20000.00	916.67
303.15	20000.00	911.72
308.15	20000.00	906.8
313.15	20000.00	901.8
318.15	20000.00	896.91
323.15	20000.00	891.93
328.15	20000.00	886.97
333.15	20000.00	881.93
338.15	20000.00	876.98
283.15	25000.00	935.19
288.15	25000.00	930.32
293.15	25000.00	925.54
298.15	25000.00	920.61
303.15	25000.00	915.8
308.15	25000.00	910.98
313.15	25000.00	906.18
318.15	25000.00	901.27
323.15	25000.00	896.47
328.15	25000.00	891.57
333.15	25000.00	886.74
338.15	25000.00	881.86
283.15	30000.00	938.66
288.15	30000.00	933.89
293.15	30000.00	929.07
298.15	30000.00	924.3
303.15	30000.00	919.58
308.15	30000.00	914.84
313.15	30000.00	910.18
318.15	30000.00	905.42
323.15	30000.00	900.65
328.15	30000.00	895.96
333.15	30000.00	891.26
338.15	30000.00	886.43
283.15	35000.00	942.04
288.15	35000.00	937.37
293.15	35000.00	932.7
298.15	35000.00	928.03
303.15	35000.00	923.37
308.15	35000.00	918.68

313.15	35000.00	914.06
318.15	35000.00	909.5
323.15	35000.00	904.8
328.15	35000.00	900.23
333.15	35000.00	895.59
338.15	35000.00	890.92
283.15	40000.00	945.33
288.15	40000.00	940.66
293.15	40000.00	936.06
298.15	40000.00	931.52
303.15	40000.00	927.0
308.15	40000.00	922.47
313.15	40000.00	917.85
318.15	40000.00	913.4
323.15	40000.00	908.8
328.15	40000.00	904.35
333.15	40000.00	899.79
338.15	40000.00	895.2
283.15	45000.00	948.5
288.15	45000.00	943.92
293.15	45000.00	939.48
298.15	45000.00	934.92
303.15	45000.00	930.47
308.15	45000.00	925.95
313.15	45000.00	921.58
318.15	45000.00	917.1
323.15	45000.00	912.67
328.15	45000.00	908.24
333.15	45000.00	903.78
338.15	45000.00	899.36
283.15	50000.00	951.53
288.15	50000.00	947.13
293.15	50000.00	942.66
298.15	50000.00	938.29
303.15	50000.00	933.84
308.15	50000.00	929.45
313.15	50000.00	925.04
318.15	50000.00	920.67
323.15	50000.00	916.35
328.15	50000.00	912.04
333.15	50000.00	907.66
338.15	50000.00	903.34
283.15	55000.00	954.61
288.15	55000.00	950.18

293.15	55000.00	945.78
298.15	55000.00	941.41
303.15	55000.00	937.1
308.15	55000.00	932.76
313.15	55000.00	928.5
318.15	55000.00	924.18
323.15	55000.00	919.97
328.15	55000.00	915.63
333.15	55000.00	911.34
338.15	55000.00	907.07
283.15	60000.00	957.6
288.15	60000.00	953.28
293.15	60000.00	948.91
298.15	60000.00	944.69
303.15	60000.00	940.35
308.15	60000.00	936.18
313.15	60000.00	931.93
318.15	60000.00	927.71
323.15	60000.00	923.48
328.15	60000.00	919.32
333.15	60000.00	915.07
338.15	60000.00	910.92
283.15	65000.00	960.38
288.15	65000.00	956.1
293.15	65000.00	951.86
298.15	65000.00	947.7
303.15	65000.00	943.48
308.15	65000.00	939.24
313.15	65000.00	935.06
318.15	65000.00	930.91
323.15	65000.00	926.81
328.15	65000.00	922.64
333.15	65000.00	918.6
338.15	65000.00	914.41

Reference

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Sources

**The Yaws Handbook of Vapor Pressure:
Crippen Method:**
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<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
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Measurement and modeling of infinite dilution activity coefficients of organic compounds in a polar ionic liquid
Comprehensive Study of the Thermophysical Properties of [Tf₂N]⁻ based ionic liquids: 1-Ethyl-3-methylimidazolium Hexafluorophosphate and 2-Ethylfuran:
NIST Webbook: <https://www.doi.org/10.1016/j.fluid.2019.01.028>
<https://www.doi.org/10.1021/acs.jced.8b00153>
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Legend

ie:	Ionization energy
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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