

2-Ethylfuran

Other names:	2-Ethylfurane Furan, «alpha»-ethyl- furan, 2-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
af	0.3065		Cheméo Relay (1.0)
hf	-100.74	kJ/mol	Cheméo Relay (1.0)
hvap	34.45	kJ/mol	Cheméo Relay (1.0)
ie	8.45 ± 0.05	eV	NIST Webbook
logp	1.842		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
pc	4033.90	kPa	Cheméo Relay (1.0, beta)
rinpol	685.81		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	694.00		NIST Webbook
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rinpol	712.00	NIST Webbook
rinpol	704.00	NIST Webbook
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rinpol	720.00	NIST Webbook
rinpol	702.00	NIST Webbook
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ripol	950.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	952.00		NIST Webbook
tb	365.65 ± 2.00	K	NIST Webbook
tb	364.00 ± 3.00	K	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
tc	548.36	K	Cheméo Relay (1.0)
vc	0.311	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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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

Sources

Measurement and modeling of infinite dilution activity coefficients of organic compounds in an equimolar ionic liquid pressure of [Bmim]Cl and [Bmim][Tf2N]: NIST Webbook:	https://www.doi.org/10.1016/j.fluid.2019.01.028 https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure http://webbook.nist.gov/cgi/cbook.cgi?ID=C3208160&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Comparative Study of the Thermophysical Properties of 2-Ethylthiophene and 2-Ethylfuran:	https://www.doi.org/10.1021/acs.jced.8b00153

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
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
tc:	Critical Temperature
vc:	Critical Volume

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