

Ethanone, 1-(2-thienyl)-

Other names:	1-(2-Thienyl)ethanone 2-ACETOTHIOPHENE 2-Acetylthiophene 2-Acethienone 2-Acetylthiophen 2-Acetylthiophene 2-Thienyl methyl ketone Ketone, methyl 2-thienyl METHYL 2-THIENYL KETONE NSC 2345 thiophene, 2-acetyl-
Inchi:	InChI=1S/C6H6OS/c1-5(7)6-3-2-4-8-6/h2-4H,1H3
InchiKey:	WYJOVVXUZNRJQY-UHFFFAOYSA-N
Formula:	C6H6OS
SMILES:	CC(=O)c1cccs1
Mol. weight [g/mol]:	126.18
CAS:	88-15-3

Physical Properties

Property code	Value	Unit	Source
cpl	205.70	J/molxK	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cpl	210.72	J/molxK	Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylfuran and 2-acetylthiophene
hvap	58.80 ± 1.20	kJ/mol	NIST Webbook
ie	9.20 ± 0.05	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.951		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1049.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1041.00		NIST Webbook

rinpol	1066.00	NIST Webbook
rinpol	1067.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1052.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1061.00	NIST Webbook
rinpol	1061.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1116.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1052.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1095.00	NIST Webbook
ripol	1731.00	NIST Webbook
ripol	1760.00	NIST Webbook
ripol	1725.00	NIST Webbook
ripol	1762.00	NIST Webbook
ripol	1740.00	NIST Webbook
ripol	1740.00	NIST Webbook
ripol	1773.00	NIST Webbook
ripol	1771.00	NIST Webbook
ripol	1777.00	NIST Webbook

ripol	1777.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1785.00		NIST Webbook
tb	486.50 ± 0.50	K	NIST Webbook
tb	486.70	K	NIST Webbook
tb	505.05	K	KDB
tf	282.00	K	NIST Webbook
tf	283.60 ± 0.02	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.70	NIST Webbook
tbrp	368.60 ± 1.00	K	1.70	NIST Webbook

Datasets

Mass density, kg/m³

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m ³ - Liquid
100.00	283.15	1180.61
100.00	288.15	1175.97
100.00	293.15	1171.0
100.00	298.15	1166.24
100.00	303.15	1161.59
100.00	308.15	1156.84
100.00	313.15	1152.05
100.00	318.15	1147.15
100.00	323.15	1142.34
100.00	328.15	1137.56
100.00	333.15	1132.76

100.00	338.15	1127.97
2000.00	283.15	1181.78
2000.00	288.15	1177.04
2000.00	293.15	1172.28
2000.00	298.15	1167.52
2000.00	303.15	1162.77
2000.00	308.15	1158.03
2000.00	313.15	1153.3
2000.00	318.15	1148.56
2000.00	323.15	1143.79
2000.00	328.15	1139.02
2000.00	333.15	1134.24
2000.00	338.15	1129.47
5000.00	283.15	1183.44
5000.00	288.15	1178.73
5000.00	293.15	1174.02
5000.00	298.15	1169.28
5000.00	303.15	1164.6
5000.00	308.15	1159.89
5000.00	313.15	1155.19
5000.00	318.15	1150.49
5000.00	323.15	1145.78
5000.00	328.15	1141.06
5000.00	333.15	1136.33
5000.00	338.15	1131.61
7000.00	283.15	1184.54
7000.00	288.15	1179.85
7000.00	293.15	1175.16
7000.00	298.15	1170.46
7000.00	303.15	1165.79
7000.00	308.15	1161.11
7000.00	313.15	1156.45
7000.00	318.15	1151.77
7000.00	323.15	1147.09
7000.00	328.15	1142.39
7000.00	333.15	1137.7
7000.00	338.15	1133.01
10000.00	283.15	1186.17
10000.00	288.15	1181.52
10000.00	293.15	1176.85
10000.00	298.15	1172.2
10000.00	303.15	1167.56
10000.00	308.15	1162.92
10000.00	313.15	1158.29

10000.00	318.15	1153.65
10000.00	323.15	1149.02
10000.00	328.15	1144.38
10000.00	333.15	1139.72
10000.00	338.15	1135.08
15000.00	283.15	1188.81
15000.00	288.15	1184.21
15000.00	293.15	1179.61
15000.00	298.15	1175.02
15000.00	303.15	1170.45
15000.00	308.15	1165.87
15000.00	313.15	1161.33
15000.00	318.15	1156.74
15000.00	323.15	1152.17
15000.00	328.15	1147.6
15000.00	333.15	1143.11
15000.00	338.15	1138.55
20000.00	283.15	1191.4
20000.00	288.15	1186.85
20000.00	293.15	1182.3
20000.00	298.15	1177.77
20000.00	303.15	1173.26
20000.00	308.15	1168.75
20000.00	313.15	1164.23
20000.00	318.15	1159.72
20000.00	323.15	1155.23
20000.00	328.15	1150.78
20000.00	333.15	1146.25
20000.00	338.15	1141.78
25000.00	283.15	1193.92
25000.00	288.15	1189.43
25000.00	293.15	1184.93
25000.00	298.15	1180.44
25000.00	303.15	1175.98
25000.00	308.15	1171.53
25000.00	313.15	1167.08
25000.00	318.15	1162.64
25000.00	323.15	1158.22
25000.00	328.15	1153.79
25000.00	333.15	1149.39
25000.00	338.15	1144.86
30000.00	283.15	1196.37
30000.00	288.15	1191.93
30000.00	293.15	1187.48

30000.00	298.15	1183.06
30000.00	303.15	1178.65
30000.00	308.15	1174.24
30000.00	313.15	1169.85
30000.00	318.15	1165.47
30000.00	323.15	1161.08
30000.00	328.15	1156.77
30000.00	333.15	1152.35
30000.00	338.15	1147.94
35000.00	283.15	1198.77
35000.00	288.15	1194.37
35000.00	293.15	1189.98
35000.00	298.15	1185.59
35000.00	303.15	1181.25
35000.00	308.15	1176.89
35000.00	313.15	1172.56
35000.00	318.15	1168.21
35000.00	323.15	1163.89
35000.00	328.15	1159.56
35000.00	333.15	1155.23
35000.00	338.15	1150.94
40000.00	283.15	1201.11
40000.00	288.15	1196.76
40000.00	293.15	1192.41
40000.00	298.15	1188.08
40000.00	303.15	1183.77
40000.00	308.15	1179.46
40000.00	313.15	1175.19
40000.00	318.15	1170.9
40000.00	323.15	1166.63
40000.00	328.15	1162.34
40000.00	333.15	1158.08
40000.00	338.15	1153.82
45000.00	283.15	1203.39
45000.00	288.15	1199.09
45000.00	293.15	1194.78
45000.00	298.15	1190.5
45000.00	303.15	1186.24
45000.00	308.15	1181.98
45000.00	313.15	1177.74
45000.00	318.15	1173.5
45000.00	323.15	1169.28
45000.00	328.15	1165.07
45000.00	333.15	1160.83

45000.00	338.15	1156.64
50000.00	293.15	1197.1
50000.00	298.15	1192.87
50000.00	303.15	1188.64
50000.00	308.15	1184.43
50000.00	313.15	1180.24
50000.00	318.15	1176.04
50000.00	323.15	1171.88
50000.00	328.15	1167.69
50000.00	333.15	1163.52
50000.00	338.15	1159.38
55000.00	293.15	1199.35
55000.00	298.15	1195.17
55000.00	303.15	1190.99
55000.00	308.15	1186.82
55000.00	313.15	1182.67
55000.00	318.15	1178.53
55000.00	323.15	1174.4
55000.00	328.15	1170.28
55000.00	333.15	1166.14
55000.00	338.15	1162.04
60000.00	293.15	1201.56
60000.00	298.15	1197.42
60000.00	303.15	1193.27
60000.00	308.15	1189.15
60000.00	313.15	1185.04
60000.00	318.15	1180.93
60000.00	323.15	1176.86
60000.00	328.15	1172.79
60000.00	333.15	1168.68
60000.00	338.15	1164.64
65000.00	293.15	1203.71
65000.00	298.15	1199.61
65000.00	303.15	1195.5
65000.00	308.15	1191.41
65000.00	313.15	1187.36
65000.00	318.15	1183.29
65000.00	323.15	1179.25
65000.00	328.15	1175.21
65000.00	333.15	1171.17
65000.00	338.15	1167.11

Reference

<https://www.doi.org/10.1016/j.fluid.2016.10.026>

Sources

Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives	https://www.doi.org/10.1016/j.tca.2005.11.024
Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylfuran and 2-acetylthiophene:	https://www.doi.org/10.1016/j.tca.2009.04.012
McGowan Method:	https://www.thermo.com/files/research/kdb/mol/mol1880.mol
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Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical study of 2-acetylthiophene: Experimental and modelled results:	https://www.doi.org/10.1016/j.fluid.2016.10.026

Legend

cpl:	Liquid phase heat capacity
hvac:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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