Thiophene, 2-methyl-

Other names:	2-Methylthiacyclopentadiene
	2-Methylthiophene
	2-methylthiacyclopentadiene (2-methylthiophene)
Inchi:	InChI=1S/C5H6S/c1-5-3-2-4-6-5/h2-4H,1H3
InchiKey:	XQQBUAPQHNYYRS-UHFFFAOYSA-N
Formula:	C5H6S
SMILES:	Cc1cccs1
Mol. weight [g/mol]:	98.17
CAS:	554-14-3

Physical Properties

Property code	Value	Unit	Source
affp	859.00	kJ/mol	NIST Webbook
basg	826.50	kJ/mol	NIST Webbook
chl	-3472.00 ± 0.75	kJ/mol	NIST Webbook
hf	84.35 ± 0.92	kJ/mol	NIST Webbook
hfl	44.60 ± 0.92	kJ/mol	NIST Webbook
hvap	38.91	kJ/mol	NIST Webbook
hvap	38.70	kJ/mol	NIST Webbook
hvap	39.80	kJ/mol	NIST Webbook
ie	8.61	eV	NIST Webbook
ie	8.59	eV	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.63 ± 0.05	eV	NIST Webbook
log10ws	-1.70		Crippen Method
logp	2.057		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4673.00	kPa	KDB
rinpol	755.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	745.00		NIST Webbook

rinpol	773.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	767.00	NIST Webbook
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rinpol	776.00	NIST Webbook
rinpol	752.00	NIST Webbook
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rinpol	753.00	NIST Webbook
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ripol	1092.00	NIST Webbook
ripol	1103.00	NIST Webbook
ripol	1098.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1098.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1100.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1103.00	NIST Webbook
ripol	1078.00	NIST Webbook
ripol	1092.00	NIST Webbook
ripol	1082.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1089.00	NIST Webbook
ripol	1102.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1106.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1090.00	NIST Webbook

ripol	1095.00		NIST Webbook
ripol	1120.50		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1097.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1090.00		NIST Webbook
sl	218.49	J/mol×K	NIST Webbook
tb	385.70	K	NIST Webbook
tb	385.80	K	NIST Webbook
tb	385.20	K	KDB
tb	386.00 ± 0.30	K	NIST Webbook
tb	385.15 ± 1.50	K	NIST Webbook
tc	606.20	K	NIST Webbook
tc	606.20	K	KDB
tf	209.77 ± 0.06	K	NIST Webbook
tf	209.80	K	KDB
tt	209.79 ± 0.05	K	NIST Webbook
tt	209.78	K	KDB
vc	0.279	m3/kmol	KDB
zc	0.2590420		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	149.83	J/mol×K	298.15	NIST Webbook
cps	97.91	J/mol×K	199.70	NIST Webbook
hfust	11.14	kJ/mol	207.79	NIST Webbook
hfust	9.47	kJ/mol	207.80	NIST Webbook
hfust	9.47	kJ/mol	207.80	NIST Webbook
hvapt	37.20	kJ/mol	357.50	NIST Webbook
hvapt	33.90	kJ/mol	385.70	NIST Webbook
hvapt	33.90	kJ/mol	385.70	KDB
hvapt	36.80	kJ/mol	353.00	NIST Webbook
hvapt	38.90	kJ/mol	343.00	NIST Webbook

pvap	69.87	kPa	373.10	Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water
pvap	209.80	kPa	413.15	Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water
rhol	1020.89	kg/m3	293.10	KDB
sfust	53.62	J/mol×K	207.79	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47469e+01
Coeff. B	-3.62706e+03
Coeff. C	-2.76980e+01
Temperature range (K), min.	278.54
Temperature range (K), max.	412.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.21177e+01
Coeff. B	-6.91971e+03
Coeff. C	-8.45277e+00

Coeff. D	5.17389e-06
Temperature range (K), min.	282.15
Temperature range (K), max.	610.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	1030.98
288.15	100.00	1025.61
293.15	100.00	1020.2
298.15	100.00	1014.79
303.15	100.00	1009.39
308.15	100.00	1003.95
313.15	100.00	998.5
318.15	100.00	993.03
323.15	100.00	987.55
328.15	100.00	982.01
333.15	100.00	976.49
338.15	100.00	970.87
283.15	2000.00	1032.44
288.15	2000.00	1027.12
293.15	2000.00	1021.76
298.15	2000.00	1016.39
303.15	2000.00	1011.03
308.15	2000.00	1005.62
313.15	2000.00	1000.23
318.15	2000.00	994.81
323.15	2000.00	989.38
328.15	2000.00	983.93
333.15	2000.00	978.46
338.15	2000.00	972.92
283.15	5000.00	1034.69
288.15	5000.00	1029.45
293.15	5000.00	1024.16
298.15	5000.00	1018.85
303.15	5000.00	1013.57
308.15	5000.00	1008.23

313.15	5000.00	1002.93
318.15	5000.00	997.59
323.15	5000.00	992.24
328.15	5000.00	986.87
333.15	5000.00	981.49
338.15	5000.00	976.06
283.15	7000.00	1036.18
288.15	7000.00	1030.97
293.15	7000.00	1025.73
298.15	7000.00	1020.48
303.15	7000.00	1015.23
308.15	7000.00	1009.96
313.15	7000.00	1004.7
318.15	7000.00	999.4
323.15	7000.00	994.11
328.15	7000.00	988.79
333.15	7000.00	983.47
338.15	7000.00	978.09
283.15	10000.00	1038.39
288.15	10000.00	1033.22
293.15	10000.00	1028.04
298.15	10000.00	1022.84
303.15	10000.00	1017.69
308.15	10000.00	1012.46
313.15	10000.00	1007.28
318.15	10000.00	1002.05
323.15	10000.00	996.84
328.15	10000.00	991.61
333.15	10000.00	986.36
338.15	10000.00	981.08
283.15	15000.00	1041.92
288.15	15000.00	1036.86
293.15	15000.00	1031.77
298.15	15000.00	1026.7
303.15	15000.00	1021.62
308.15	15000.00	1016.53
313.15	15000.00	1011.45
318.15	15000.00	1006.33
323.15	15000.00	1001.25
328.15	15000.00	996.12
333.15	15000.00	991.02
338.15	15000.00	985.87
283.15	20000.00	1045.36
288.15	20000.00	1040.39

293.15	20000.00	1035.39
298.15	20000.00	1030.4
303.15	20000.00	1025.42
308.15	20000.00	1020.43
313.15	20000.00	1015.45
318.15	20000.00	1010.45
323.15	20000.00	1005.47
328.15	20000.00	1000.47
333.15	20000.00	995.46
338.15	20000.00	990.45
283.15	25000.00	1048.69
288.15	25000.00	1043.79
293.15	25000.00	1038.88
298.15	25000.00	1033.98
303.15	25000.00	1029.11
308.15	25000.00	1024.2
313.15	25000.00	1019.32
318.15	25000.00	1014.42
323.15	25000.00	1009.52
328.15	25000.00	1004.64
333.15	25000.00	999.74
338.15	25000.00	994.85
283.15	30000.00	1051.93
288.15	30000.00	1047.1
293.15	30000.00	1042.27
298.15	30000.00	1037.45
303.15	30000.00	1032.66
308.15	30000.00	1027.84
313.15	30000.00	1023.04
318.15	30000.00	1018.23
323.15	30000.00	1013.45
328.15	30000.00	1008.65
333.15	30000.00	1003.86
338.15	30000.00	999.06
283.15	35000.00	1055.07
288.15	35000.00	1050.32
293.15	35000.00	1045.56
298.15	35000.00	1040.82
303.15	35000.00	1036.1
308.15	35000.00	1031.36
313.15	35000.00	1026.65
318.15	35000.00	1021.93
323.15	35000.00	1017.21
328.15	35000.00	1012.52

333.15	35000.00	1007.82
338.15	35000.00	1003.09
283.15	40000.00	1058.12
288.15	40000.00	1053.43
293.15	40000.00	1048.68
298.15	40000.00	1044.09
303.15	40000.00	1039.44
308.15	40000.00	1034.78
313.15	40000.00	1030.14
318.15	40000.00	1025.49
323.15	40000.00	1020.87
328.15	40000.00	1016.24
333.15	40000.00	1011.63
338.15	40000.00	1007.02
283.15	45000.00	1061.09
288.15	45000.00	1056.47
293.15	45000.00	1051.85
298.15	45000.00	1047.25
303.15	45000.00	1042.68
308.15	45000.00	1038.08
313.15	45000.00	1033.52
318.15	45000.00	1028.94
323.15	45000.00	1024.41
328.15	45000.00	1019.86
333.15	45000.00	1015.34
338.15	45000.00	1010.79
283.15	50000.00	1063.97
288.15	50000.00	1059.42
293.15	50000.00	1054.87
298.15	50000.00	1050.33
303.15	50000.00	1045.81
308.15	50000.00	1041.29
313.15	50000.00	1036.79
318.15	50000.00	1032.3
323.15	50000.00	1027.81
328.15	50000.00	1023.37
333.15	50000.00	1018.9
338.15	50000.00	1014.44
283.15	55000.00	1066.8
288.15	55000.00	1062.27
293.15	55000.00	1057.79
298.15	55000.00	1053.31
303.15	55000.00	1048.89
308.15	55000.00	1044.4

313.15	55000.00	1039.99
318.15	55000.00	1035.54
323.15	55000.00	1031.14
328.15	55000.00	1026.73
333.15	55000.00	1022.36
338.15	55000.00	1017.97
283.15	60000.00	1069.53
288.15	60000.00	1065.07
293.15	60000.00	1060.64
298.15	60000.00	1056.23
303.15	60000.00	1051.84
308.15	60000.00	1047.43
313.15	60000.00	1043.07
318.15	60000.00	1038.69
323.15	60000.00	1034.36
328.15	60000.00	1030.01
333.15	60000.00	1025.71
338.15	60000.00	1021.38
283.15	65000.00	1072.21
288.15	65000.00	1067.79
293.15	65000.00	1063.42
298.15	65000.00	1059.07
303.15	65000.00	1054.72
308.15	65000.00	1050.39
313.15	65000.00	1046.08
318.15	65000.00	1041.75
323.15	65000.00	1037.48
328.15	65000.00	1033.2
333.15	65000.00	1028.94
338.15	65000.00	1024.7

Reference *https://www.doi.org/10.1016/j.jct.2016.08.005*

Sources

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Removal of 2- and 3-methylthiophene from their mixtures with n-heptane using tetrahexylammonium bromide-based deep eutectic solvents as extractive desulfurization agents:	https://www.doi.org/10.1016/j.jct.2018.05.026
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NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C554143&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility