Thiophene, 3-methyl-

Other names:	.beta.-methylthiophene
	3-Methylthiophene
	3-THIOTOLENE
	Methyl-3-thiophene
	«beta»-Methylthiophene
	Â«betaÂ»-Methylthiophene
Inchi:	InChI=1S/C5H6S/c1-5-2-3-6-4-5/h2-4H,1H3
InchiKey:	QENGPZGAWFQWCZ-UHFFFAOYSA-N
Formula:	C5H6S
SMILES:	Cc1ccsc1
Mol. weight [g/mol]:	98.17
CAS:	616-44-4

Physical Properties

Property code	Value	Unit	Source
chl	-3470.40 ± 0.71	kJ/mol	NIST Webbook
hf	82.59 ± 0.92	kJ/mol	NIST Webbook
hfl	43.05 ± 0.88	kJ/mol	NIST Webbook
hvap	39.50	kJ/mol	NIST Webbook
hvap	39.50	kJ/mol	NIST Webbook
hvap	39.46	kJ/mol	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.84	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.39		Aqueous Solubility Prediction Method
logp	2.057		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4788.00	kPa	KDB
rinpol	760.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	786.00		NIST Webbook

rinpol	790.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	805.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	757.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1120.00	NIST Webbook
ripol	1136.00	NIST Webbook
ripol	1106.00	NIST Webbook
ripol	1136.00	NIST Webbook
ripol	1127.00	NIST Webbook

ripol	1123.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1099.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1117.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1115.00		NIST Webbook
tb	388.60	K	KDB
tb	388.60 ± 0.30	K	NIST Webbook
tb	388.60	K	NIST Webbook
tb	388.35	K	Isobaric vapor-liquid equilibrium for four binary systems of 3-methylthiophene
tb	388.60	K	NIST Webbook
tb	388.35	K	Isobaric vapor-liquid equilibrium for systems containing sulfur compounds
tc	610.80	K	KDB
tc	610.80	K	NIST Webbook
tf	204.20	K	KDB
tf	204.21 ± 0.06	K	NIST Webbook
tt	204.19 ± 0.02	K	NIST Webbook
tt	204.18	K	KDB
vc	0.275	m3/kmol	KDB
zc	0.2590810		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	10.54	kJ/mol	204.20	NIST Webbook
hfust	10.54	kJ/mol	204.20	NIST Webbook
hvapt	36.80	kJ/mol	362.00	NIST Webbook
hvapt	34.25	kJ/mol	388.60	KDB
hvapt	34.24	kJ/mol	388.60	NIST Webbook
hvapt	37.30	kJ/mol	360.50	NIST Webbook
hvapt	37.50	kJ/mol	363.00	NIST Webbook
hvapt	37.40	kJ/mol	353.00	NIST Webbook
hvapt	39.50	kJ/mol	329.00	NIST Webbook
rfi	1.51720		298.15	Phase equilibria on four binary systems containing 3-methylthiophene
rfi	1.51720		298.15	Phase equilibria of binary systems of 3-methylthiophene with four different hydrocarbons
rhol	1020.89	kg/m3	293.10	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	98.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45884e+01
Coeff. B	-3.49514e+03
Coeff. C	-3.80360e+01

Temperature range (K), min.	282.44
Temperature range (K), max.	414.79

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.19136e+01
Coeff. B	-6.97496e+03
Coeff. C	-8.40512e+00
Coeff. D	5.04996e-06
Temperature range (K), min.	284.15
Temperature range (K), max.	615.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	1031.82
288.15	100.00	1026.57
293.15	100.00	1021.31
298.15	100.00	1016.0
303.15	100.00	1010.72
308.15	100.00	1005.4
313.15	100.00	1000.05
318.15	100.00	994.7
323.15	100.00	989.3
328.15	100.00	983.88
333.15	100.00	978.47
338.15	100.00	972.98
283.15	2000.00	1033.26
288.15	2000.00	1028.05
293.15	2000.00	1022.81
298.15	2000.00	1017.57
303.15	2000.00	1012.32
308.15	2000.00	1007.04
313.15	2000.00	1001.76
318.15	2000.00	996.44

323.15	2000.00	991.1
328.15	2000.00	985.74
333.15	2000.00	980.39
338.15	2000.00	974.96
283.15	5000.00	1035.47
288.15	5000.00	1030.34
293.15	5000.00	1025.16
298.15	5000.00	1019.98
303.15	5000.00	1014.81
308.15	5000.00	1009.61
313.15	5000.00	1004.39
318.15	5000.00	999.15
323.15	5000.00	993.9
328.15	5000.00	988.63
333.15	5000.00	983.35
338.15	5000.00	978.01
283.15	7000.00	1036.93
288.15	7000.00	1031.84
293.15	7000.00	1026.7
298.15	7000.00	1021.56
303.15	7000.00	1016.43
308.15	7000.00	1011.27
313.15	7000.00	1006.11
318.15	7000.00	1000.93
323.15	7000.00	995.72
328.15	7000.00	990.51
333.15	7000.00	985.3
338.15	7000.00	980.02
283.15	10000.00	1039.07
288.15	10000.00	1034.03
293.15	10000.00	1028.95
298.15	10000.00	1023.89
303.15	10000.00	1018.83
308.15	10000.00	1013.72
313.15	10000.00	1008.64
318.15	10000.00	1003.52
323.15	10000.00	998.41
328.15	10000.00	993.26
333.15	10000.00	988.13
338.15	10000.00	982.95
283.15	15000.00	1042.56
288.15	15000.00	1037.61
293.15	15000.00	1032.61
298.15	15000.00	1027.64

303.15	15000.00	1022.7
308.15	15000.00	1017.69
313.15	15000.00	1012.71
318.15	15000.00	1007.7
323.15	15000.00	1002.71
328.15	15000.00	997.7
333.15	15000.00	992.67
338.15	15000.00	987.63
283.15	20000.00	1045.93
288.15	20000.00	1041.07
293.15	20000.00	1036.16
298.15	20000.00	1031.29
303.15	20000.00	1026.42
308.15	20000.00	1021.53
313.15	20000.00	1016.63
318.15	20000.00	1011.74
323.15	20000.00	1006.85
328.15	20000.00	1001.93
333.15	20000.00	997.03
338.15	20000.00	992.12
283.15	25000.00	1049.2
288.15	25000.00	1044.41
293.15	25000.00	1039.6
298.15	25000.00	1034.81
303.15	25000.00	1030.01
308.15	25000.00	1025.22
313.15	25000.00	1020.43
318.15	25000.00	1015.6
323.15	25000.00	1010.83
328.15	25000.00	1006.0
333.15	25000.00	1001.22
338.15	25000.00	996.41
283.15	30000.00	1052.37
288.15	30000.00	1047.65
293.15	30000.00	1042.92
298.15	30000.00	1038.2
303.15	30000.00	1033.5
308.15	30000.00	1028.73
313.15	30000.00	1024.08
318.15	30000.00	1019.35
323.15	30000.00	1014.66
328.15	30000.00	1009.94
333.15	30000.00	1005.22
338.15	30000.00	1000.53

283.15	35000.00	1055.46
288.15	35000.00	1050.8
293.15	35000.00	1046.15
298.15	35000.00	1041.52
303.15	35000.00	1036.87
308.15	35000.00	1032.24
313.15	35000.00	1027.61
318.15	35000.00	1022.99
323.15	35000.00	1018.35
328.15	35000.00	1013.73
333.15	35000.00	1009.12
338.15	35000.00	1004.49
283.15	40000.00	1058.46
288.15	40000.00	1053.86
293.15	40000.00	1049.27
298.15	40000.00	1044.71
303.15	40000.00	1040.16
308.15	40000.00	1035.59
313.15	40000.00	1031.05
318.15	40000.00	1026.48
323.15	40000.00	1021.93
328.15	40000.00	1017.38
333.15	40000.00	1012.87
338.15	40000.00	1008.33
283.15	45000.00	1061.37
288.15	45000.00	1056.84
293.15	45000.00	1052.31
298.15	45000.00	1047.82
303.15	45000.00	1043.34
308.15	45000.00	1038.84
313.15	45000.00	1034.35
318.15	45000.00	1029.86
323.15	45000.00	1025.4
328.15	45000.00	1020.94
333.15	45000.00	1016.49
338.15	45000.00	1012.04
283.15	50000.00	1064.22
288.15	50000.00	1059.74
293.15	50000.00	1055.28
298.15	50000.00	1050.84
303.15	50000.00	1046.42
308.15	50000.00	1041.98
313.15	50000.00	1037.58
318.15	50000.00	1033.15

323.15	50000.00	1028.76
328.15	50000.00	1024.36
333.15	50000.00	1020.0
338.15	50000.00	1015.62
283.15	55000.00	1066.97
288.15	55000.00	1062.56
293.15	55000.00	1058.15
298.15	55000.00	1053.78
303.15	55000.00	1049.41
308.15	55000.00	1045.05
313.15	55000.00	1040.71
318.15	55000.00	1036.33
323.15	55000.00	1032.03
328.15	55000.00	1027.68
333.15	55000.00	1023.38
338.15	55000.00	1019.08
283.15	60000.00	1069.67
288.15	60000.00	1065.32
293.15	60000.00	1060.96
298.15	60000.00	1056.65
303.15	60000.00	1052.33
308.15	60000.00	1048.03
313.15	60000.00	1043.73
318.15	60000.00	1039.44
323.15	60000.00	1035.18
328.15	60000.00	1030.89
333.15	60000.00	1026.67
338.15	60000.00	1022.44
283.15	65000.00	1072.32
288.15	65000.00	1068.01
293.15	65000.00	1063.7
298.15	65000.00	1059.43
303.15	65000.00	1055.16
308.15	65000.00	1050.91
313.15	65000.00	1046.69
318.15	65000.00	1042.45
323.15	65000.00	1038.24
328.15	65000.00	1034.03
333.15	65000.00	1029.88
338.15	65000.00	1025.7

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

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KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1874
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Phase equilibria on four binary systems containing 3-methylthiophene:	https://www.doi.org/10.1016/j.fluid.2009.02.010

Legend

chl:	Standard liquid enthalpy of combustion
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
rfi:	Refractive Index
rhol:	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
tf:	Normal melting (fusion) point

tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility