Thiophene, 2,5-dimethyl-

Other names: 2,5-Dimethylthiophene
Inchi: InChI=1S/C6H8S/c1-5-3-4-6(2)7-5/h3-4H,1-2H3
InchiKey: GWQOOADXMVQEFT-UHFFFAOYSA-N
Formula: C6H8S
SMILES: Cc1ccc(C)s1
Mol. weight [g/mol]: 112.19
CAS: 638-02-8

Physical Properties

Property code	Value	Unit	Source
hvap	40.20 ± 0.90	kJ/mol	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.365		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
pc	3890.00	kPa	KDB
rinpol	856.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	850.00		NIST Webbook

rinpol	856.00	NIST Webbook
rinpol	876.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	878.00	NIST Webbook
rinpol	874.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	845.00	NIST Webbook
rinpol	905.00	NIST Webbook
rinpol	876.00	NIST Webbook
rinpol	866.00	NIST Webbook
rinpol	868.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	845.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	877.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	855.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	863.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	852.00	NIST Webbook
rinpol	852.00	NIST Webbook
ripol	1179.00	NIST Webbook
ripol	1178.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1156.00	NIST Webbook
ripol	1190.00	NIST Webbook
ripol	1187.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1187.00	NIST Webbook
ripol	1166.00	NIST Webbook
ripol	1190.00	NIST Webbook

ripol	1167.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1202.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1168.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1165.00		NIST Webbook
sl	244.72	J/mol×K	NIST Webbook
tb	409.90	K	KDB
tb	409.70	K	NIST Webbook
tb	409.96	K	Phase equilibria of three binary systems containing 2,5-dimethylthiophene and 2-ethylthiophene in hydrocarbons
tc	625.20	K	KDB
tf	210.60	K	KDB
tt	204.87 ± 0.06	K	NIST Webbook
tt	210.58 ± 0.03	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	178.32	J/mol×K	298.15	NIST Webbook
hfust	8.91	kJ/mol	210.60	NIST Webbook
hfust	8.91	kJ/mol	210.60	NIST Webbook
hvapt	39.70	kJ/mol	353.50	NIST Webbook
pvap	101.33	kPa	409.96	Phase equilibria of three binary systems containing 2,5-dimethylthiophene and 2-ethylthiophene in hydrocarbons
rhol	987.26	kg/m3	293.10	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.20	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47339e+01
Coeff. B	-3.80718e+03
Coeff. C	-3.33330e+01
Temperature range (K), min.	296.87
Temperature range (K), max.	437.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.01211e+01
Coeff. B	-5.38395e+03
Coeff. C	-2.08877e+00
Coeff. D	1.43521e-06
Temperature range (K), min.	333.15
Temperature range (K), max.	374.15

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	995.51
288.15	100.00	990.41
293.15	100.00	985.3
298.15	100.00	980.2
303.15	100.00	975.1

308.15	100.00	970.0
313.15	100.00	964.84
318.15	100.00	959.75
323.15	100.00	954.64
328.15	100.00	949.46
333.15	100.00	944.28
338.15	100.00	939.09
283.15	2000.00	996.96
288.15	2000.00	991.9
293.15	2000.00	986.82
298.15	2000.00	981.78
303.15	2000.00	976.72
308.15	2000.00	971.66
313.15	2000.00	966.6
318.15	2000.00	961.52
323.15	2000.00	956.46
328.15	2000.00	951.34
333.15	2000.00	946.2
338.15	2000.00	941.08
283.15	5000.00	999.21
288.15	5000.00	994.21
293.15	5000.00	989.21
298.15	5000.00	984.2
303.15	5000.00	979.23
308.15	5000.00	974.22
313.15	5000.00	969.22
318.15	5000.00	964.24
323.15	5000.00	959.26
328.15	5000.00	954.21
333.15	5000.00	949.16
338.15	5000.00	944.14
283.15	7000.00	1000.68
288.15	7000.00	995.72
293.15	7000.00	990.74
298.15	7000.00	985.8
303.15	7000.00	980.88
308.15	7000.00	975.91
313.15	7000.00	970.97
318.15	7000.00	966.0
323.15	7000.00	961.09
328.15	7000.00	956.1
333.15	7000.00	951.09
338.15	7000.00	946.13
283.15	10000.00	1002.83

288.15	10000.00	997.94
293.15	10000.00	993.02
298.15	10000.00	988.14
303.15	10000.00	983.27
308.15	10000.00	978.38
313.15	10000.00	973.5
318.15	10000.00	968.6
323.15	10000.00	963.75
328.15	10000.00	958.85
333.15	10000.00	953.92
338.15	10000.00	949.02
283.15	15000.00	1006.35
288.15	15000.00	1001.53
293.15	15000.00	996.71
298.15	15000.00	991.93
303.15	15000.00	987.17
308.15	15000.00	982.36
313.15	15000.00	977.58
318.15	15000.00	972.8
323.15	15000.00	968.05
328.15	15000.00	963.27
333.15	15000.00	958.46
338.15	15000.00	953.67
283.15	20000.00	1009.74
288.15	20000.00	1005.01
293.15	20000.00	1000.28
298.15	20000.00	995.59
303.15	20000.00	990.9
308.15	20000.00	986.2
313.15	20000.00	981.52
318.15	20000.00	976.83
323.15	20000.00	972.19
328.15	20000.00	967.5
333.15	20000.00	962.79
338.15	20000.00	958.14
283.15	25000.00	1013.04
288.15	25000.00	1008.38
293.15	25000.00	1003.72
298.15	25000.00	999.13
303.15	25000.00	994.52
308.15	25000.00	989.91
313.15	25000.00	985.31
318.15	25000.00	980.72
323.15	25000.00	976.16

328.15	25000.00	971.57
333.15	25000.00	966.97
338.15	25000.00	962.41
283.15	30000.00	1016.24
288.15	30000.00	1011.66
293.15	30000.00	1007.07
298.15	30000.00	1002.53
303.15	30000.00	998.02
308.15	30000.00	993.47
313.15	30000.00	988.97
318.15	30000.00	984.44
323.15	30000.00	979.99
328.15	30000.00	975.49
333.15	30000.00	970.97
338.15	30000.00	966.51
283.15	35000.00	1019.33
288.15	35000.00	1014.81
293.15	35000.00	1010.31
298.15	35000.00	1005.84
303.15	35000.00	1001.4
308.15	35000.00	996.93
313.15	35000.00	992.49
318.15	35000.00	988.06
323.15	35000.00	983.67
328.15	35000.00	979.25
333.15	35000.00	974.83
338.15	35000.00	970.46
283.15	40000.00	1022.34
288.15	40000.00	1017.89
293.15	40000.00	1013.45
298.15	40000.00	1009.04
303.15	40000.00	1004.69
308.15	40000.00	1000.28
313.15	40000.00	995.92
318.15	40000.00	991.55
323.15	40000.00	987.24
328.15	40000.00	982.9
333.15	40000.00	978.55
338.15	40000.00	974.25
283.15	45000.00	1025.27
288.15	45000.00	1020.88
293.15	45000.00	1016.49
298.15	45000.00	1012.17
303.15	45000.00	1007.85

308.15	45000.00	1003.53
313.15	45000.00	999.23
318.15	45000.00	994.93
323.15	45000.00	990.69
328.15	45000.00	986.42
333.15	45000.00	982.15
338.15	45000.00	977.91
283.15	50000.00	1028.12
288.15	50000.00	1023.78
293.15	50000.00	1019.47
298.15	50000.00	1015.2
303.15	50000.00	1010.94
308.15	50000.00	1006.66
313.15	50000.00	1002.44
318.15	50000.00	998.2
323.15	50000.00	994.03
328.15	50000.00	989.84
333.15	50000.00	985.62
338.15	50000.00	981.46
283.15	55000.00	1030.9
288.15	55000.00	1026.62
293.15	55000.00	1022.35
298.15	55000.00	1018.14
303.15	55000.00	1013.93
308.15	55000.00	1009.75
313.15	55000.00	1005.56
318.15	55000.00	1001.39
323.15	55000.00	997.27
328.15	55000.00	993.13
333.15	55000.00	988.98
338.15	55000.00	984.88
283.15	60000.00	1033.6
288.15	60000.00	1029.38
293.15	60000.00	1025.15
298.15	60000.00	1021.01
303.15	60000.00	1016.85
308.15	60000.00	1012.72
313.15	60000.00	1008.58
318.15	60000.00	1004.46
323.15	60000.00	1000.41
328.15	60000.00	996.35
333.15	60000.00	992.25
338.15	60000.00	988.2
283.15	65000.00	1036.24

288.15	65000.00	1032.06
293.15	65000.00	1027.88
298.15	65000.00	1023.8
303.15	65000.00	1019.68
308.15	65000.00	1015.59
313.15	65000.00	1011.53
318.15	65000.00	1007.46
323.15	65000.00	1003.46
328.15	65000.00	999.44
333.15	65000.00	995.41
338.15	65000.00	991.43

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Legend

cpl: Liquid phase heat capacity
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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature