Thiophene, 3,4-dimethyl-

Other names: 3,4-Dimethylthiophene
Inchi: InChI=1S/C6H8S/c1-5-3-7-4-6(5)2/h3-4H,1-2H3
InchiKey: GPSFYJDZKSRMKZ-UHFFFAOYSA-N
Formula: C6H8S
SMILES: Cc1cscc1C
Mol. weight [g/mol]: 112.19
CAS: 632-15-5

Physical Properties

Property code	Value	Unit	Source
ie	8.55	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.365		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
pc	3908.00	kPa	KDB
rinpol	890.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	908.10		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	883.50		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	883.00		NIST Webbook

rinpol	908.10		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	888.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1250.00		NIST Webbook
tb	418.20	K	KDB
tb	418.20	K	NIST Webbook
tc	640.20	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	41.10	kJ/mol	403.00	NIST Webbook
rhol	1009.70	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42237e+01
Coeff. B	-3.42431e+03
Coeff. C	-6.17000e+01
Temperature range (K), min.	307.42
Temperature range (K), max.	445.93

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.23984e+01
Coeff. B	-7.87240e+03
Coeff. C	-9.93415e+00
Coeff. D	5.82356e-06

Temperature range (K), min.	328.15
Temperature range (K), max.	478.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1885.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C632155&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1885

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature