Thiophene, 2,3-dimethyl-

Other names: 2,3-Dimethylthiophene
Inchi: InChI=1S/C6H8S/c1-5-3-4-7-6(5)2/h3-4H,1-2H3
InchiKey: BZYUMXXOAYSFOW-UHFFFAOYSA-N
Formula: C6H8S
SMILES: Cc1ccsc1C
Mol. weight [g/mol]: 112.19
CAS: 632-16-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	2.365		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
rinpol	870.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	869.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1221.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1203.00		NIST Webbook
tb	413.70 ± 2.00	K	NIST Webbook
tb	414.40 ± 3.00	K	NIST Webbook
tf	224.20 ± 0.60	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	39.40	kJ/mol	413.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43203e+01
Coeff. B	-3.42135e+03
Coeff. C	-6.10540e+01
Temperature range (K), min.	304.87
Temperature range (K), max.	440.83

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1882.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C632166&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pvap: Vapor pressure

rinpol: Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point