Thiophene, 2,3,4-trimethyl-

Other names: 2,3,4-Trimethylthiophene
Inchi: InChI=1S/C7H10S/c1-5-4-8-7(3)6(5)2/h4H,1-3H3
InchiKey: MAVVDCDMBKFUES-UHFFFAOYSA-N
Formula: C7H10S
SMILES: Cc1csc(C)c1C
Mol. weight [g/mol]: 126.22
CAS: 1795-04-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.673		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	982.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	993.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60432e+01
Coeff. B	-4.17666e+03
Coeff. C	-6.69630e+01
Temperature range (K), min.	332.05
Temperature range (K), max.	456.15

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795046&Units=SI

Legend

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