

Tetramethylthiophene

Other names:	2,3,4,5-Tetramethylthiophene Thiophene,tetramethyl-
Inchi:	InChI=1S/C8H12S/c1-5-6(2)8(4)9-7(5)3/h1-4H3
InchiKey:	IYULAUPEFMQEKK-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	Cc1sc(C)c(C)c1C
Mol. weight [g/mol]:	140.25
CAS:	14503-51-6

Physical Properties

Property code	Value	Unit	Source
ie	7.93	eV	NIST Webbook
log10ws	-3.13		Crippen Method
logp	2.982		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1100.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook

Sources

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=C14503516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/61-146-2/Tetramethylthiophene.pdf>

Generated by Cheméo on 2024-04-30 17:16:51.664635855 +0000 UTC m=+16786660.585213165.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.