# Tetramethylthiophene

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|---|---|
| **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

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|---|---|
| **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/ci990307l |

# Legend

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

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