

# 3-Ethyl-4-methylthiophene

<b>Other names:</b>	Thiophene, 3-ethyl-4-methyl-
<b>Inchi:</b>	InChI=1S/C7H10S/c1-3-7-5-8-4-6(7)2/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	QMHNYDJBWOPGHE-UHFFFAOYSA-N
<b>Formula:</b>	C7H10S
<b>SMILES:</b>	CCc1csc1C
<b>Mol. weight [g/mol]:</b>	126.22
<b>CAS:</b>	66577-03-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	2.619		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	958.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	958.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C66577035&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C66577035&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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