

Thiophene, 5-ethyl-2,3-dimethyl

Other names:	5-Ethyl-2,3-dimethylthiophene
Inchi:	InChI=1S/C8H12S/c1-4-8-5-6(2)7(3)9-8/h5H,4H2,1-3H3
InchiKey:	WFOUEDZBEUPAPA-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CCc1cc(C)c(C)s1
Mol. weight [g/mol]:	140.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.927		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1055.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1056.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41897&Units=SI
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

Legend

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

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<https://www.chemeo.com/cid/53-480-0/Thiophene-5-ethyl-2-3-dimethyl.pdf>

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