

2-Ethyl-4-methylthiophene

Other names:	Thiophene, 2-ethyl-4-methyl
Inchi:	InChI=1S/C7H10S/c1-3-7-4-6(2)5-8-7/h4-5H,3H2,1-2H3
InchiKey:	NZOYEHXPXDWJOCN-UHFFFAOYSA-N
Formula:	C7H10S
SMILES:	CCc1cc(C)cs1
Mol. weight [g/mol]:	126.22

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	955.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	953.00		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=R41815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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