

Thiophene, 2-butyl-4-methyl

Other names:	2-Butyl-4-methylthiophene
Inchi:	InChI=1S/C9H14S/c1-3-4-5-9-6-8(2)7-10-9/h6-7H,3-5H2,1-2H3
InchiKey:	NHHCUNRJYBISDA-UHFFFAOYSA-N
Formula:	C9H14S
SMILES:	CCCCc1cc(C)cs1
Mol. weight [g/mol]:	154.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	3.399		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
rinpol	1142.00		NIST Webbook
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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=R41758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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