

Thiophene, 2,4-diethyl

Other names:	2,4-Diethyl-thiophene
Inchi:	InChI=1S/C8H12S/c1-3-7-5-8(4-2)9-6-7/h5-6H,3-4H2,1-2H3
InchiKey:	DBTZOIMPUSTZCD-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CCc1csc(CC)c1
Mol. weight [g/mol]:	140.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	2.873		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
ripol	1355.00		NIST Webbook
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Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R258958&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/79-069-9/Thiophene-2-4-diethyl.pdf>

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