

Thiophene, 2,5-diethyl-

Other names:	2,5-Diethylthiophene
Inchi:	InChI=1S/C8H12S/c1-3-7-5-6-8(4-2)9-7/h5-6H,3-4H2,1-2H3
InchiKey:	JQTZGXZYJIJECF-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CCc1ccc(CC)s1
Mol. weight [g/mol]:	140.25
CAS:	5069-23-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	2.873		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1017.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C5069238&Units=SI

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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