

Thiazole, 2,5-diethyl-

Other names:	2,5-Diethylthiazole
Inchi:	InChI=1S/C7H11NS/c1-3-6-5-8-7(4-2)9-6/h5H,3-4H2,1-2H3
InchiKey:	PATFUZGQWONVOC-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	CCc1cnc(CC)s1
Mol. weight [g/mol]:	141.23
CAS:	15729-76-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	2.268		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
ripol	1090.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1463.00		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=C15729767&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
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/37-334-0/Thiazole-2-5-diethyl.pdf>

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