Thiazole, 2,4-diethyl-

Other names: 2,4-Diethylthiazole
Inchi: InChI=1S/C7H11NS/c1-3-6-5-9-7(4-2)8-6/h5H,3-4H2,1-2H3
InchiKey: IAEOVWDULPWPSJ-UHFFFAOYSA-N
Formula: C7H11NS
SMILES: CCc1csc(CC)n1
Mol. weight [g/mol]: 141.23
CAS: 32272-49-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	2.268		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1052.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1409.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32272494&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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