2,4-Diethyl-5-methylthiazole

Other names:	Thiazole, 2,4-diethyl-5-methyl-
Inchi:	InChI=1S/C8H13NS/c1-4-7-6(3)10-8(5-2)9-7/h4-5H2,1-3H3
InchiKey:	IFFHSVJYMHLVLT-UHFFFAOYSA-N
Formula:	C8H13NS
SMILES:	CCc1nc(CC)c(C)s1
Mol. weight [g/mol]:	155.26
CAS:	52414-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.576		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook

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=C52414898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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