Thiazole, 5-ethyl-2-methyl-

Other names:	5-Ethyl-2-methyl-1,3-thiazole
	2-methyl-5-ethylthiazole
	5-Ethyl-2-methylthiazole
Inchi:	InChI=1S/C6H9NS/c1-3-6-4-7-5(2)8-6/h4H,3H2,1-2H3
InchiKey:	JIZHATVFRZONHT-UHFFFAOYSA-N
Formula:	C6H9NS
SMILES:	CCc1cnc(C)s1
Mol. weight [g/mol]:	127.21
CAS:	19961-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	2.014		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	1010.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1022.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1403.00		NIST Webbook

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=C19961525&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

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