2-Methyl-5-propylthiazole

Other names:	Thiazole, 2-methyl-5-propyl
Inchi:	InChI=1S/C7H11NS/c1-3-4-7-5-8-6(2)9-7/h5H,3-4H2,1-2H3
InchiKey:	FAYMHHGWOJBXAQ-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	CCCc1cnc(C)s1
Mol. weight [g/mol]:	141.23
CAS:	52414-83-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.404		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1053.00		NIST Webbook
ripol	1418.00		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=C52414832&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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