

Thiazole, 5-methyl-2-propyl

Other names:	5-methyl-2-propylthiazole
Inchi:	InChI=1S/C7H11NS/c1-3-4-7-8-5-6(2)9-7/h5H,3-4H2,1-2H3
InchiKey:	WRHYOYIOVMOZCU-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	CCCC1ncc(C)s1
Mol. weight [g/mol]:	141.23

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	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1089.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1463.00		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=R217417&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

ripol: Polar retention indices

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