

2-Propylthiazole

Other names:	2-n-Propylthiazole Thiazole, 2-propyl-
Inchi:	InChI=1S/C6H9NS/c1-2-3-6-7-4-5-8-6/h4-5H,2-3H2,1H3
InchiKey:	CMOIEFFAOUQJPS-UHFFFAOYSA-N
Formula:	C6H9NS
SMILES:	CCc1nccs1
Mol. weight [g/mol]:	127.21
CAS:	17626-75-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	2.096		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	981.00		NIST Webbook
rinpol	969.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1381.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626754&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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