2-Propyl-4-methylthiazole

Other names: 4-Methyl-2-propylthiazole
Thiazole, 4-methyl-2-propyl-
Inchi: InChI=1S/C7H11NS/c1-3-4-7-8-6(2)5-9-7/h5H,3-4H2,1-2H3
InchiKey: WUISKNCHCVXERE-UHFFFAOYSA-N
Formula: C7H11NS
SMILES: CCCc1nc(C)cs1
Mol. weight [g/mol]: 141.23
CAS: 52414-87-6

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
rinpol	1053.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1400.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52414876&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