Thiazole, 2-methyl-4-propyl-

Other names: 2-Methyl-4-propylthiazole
Inchi: InChI=1S/C7H11NS/c1-3-4-7-5-9-6(2)8-7/h5H,3-4H2,1-2H3
InchiKey: KPTRSWJGYUCLLM-UHFFFAOYSA-N
Formula: C7H11NS
SMILES: CCCc1csc(C)n1
Mol. weight [g/mol]: 141.23
CAS: 41981-63-9

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	1085.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1428.00		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=C41981639&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