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]: 141.24

Physical Properties

Property code	Value	Unit	Source
logp	2.404		Crippen Method
mcvol	116.360	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52414832&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume