Thiazole, 2-ethyl-4-methyl-5-propyl

Inchi: InChI=1S/C10H16S/c1-4-6-10-8(3)7-9(5-2)11-10/h7H,4-6H2,1-3H3
InchiKey: PRMDWPKDNIYPJA-UHFFFAOYSA-N
Formula: C10H16S
SMILES: CCCc1sc(CC)cc1C
Mol. weight [g/mol]: 168.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	3.571		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1224.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1567.00		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=R61817&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