5-ethyl-2-isobutyl-4-methyl-thiazole

Inchi: InChI=1S/C10H17NS/c1-5-9-8(4)11-10(12-9)6-7(2)3/h7H,5-6H2,1-4H3
InchiKey: SAHLDDQDGBVGBC-UHFFFAOYSA-N
Formula: C10H17NS
SMILES: CCc1sc(CC(C)C)nc1C
Mol. weight [g/mol]: 183.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	3.212		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinpol	1297.00		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=R498250&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