

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

Inchi: InChI=1S/C9H15NS/c1-4-6-8-9(5-2)11-7(3)10-8/h4-6H2,1-3H3
InchiKey: YTFYPHBAFRPICF-UHFFFAOYSA-N
Formula: C9H15NS
SMILES: CCCc1nc(C)sc1CC
Mol. weight [g/mol]: 169.29
CAS: 4276-67-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.966		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1233.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1567.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4276679&Units=SI>
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>

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

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