

5-Ethyl-2-propylthiazole

Inchi: InChI=1S/C8H13NS/c1-3-5-8-9-6-7(4-2)10-8/h6H,3-5H2,1-2H3
InchiKey: FFSVZIJNSJWNNS-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: CCCc1ncc(CC)s1
Mol. weight [g/mol]: 155.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	2.658		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1165.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1190.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R180508&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

Latest version available from:

<https://www.chemeo.com/cid/24-043-7/5-Ethyl-2-propylthiazole.pdf>

Generated by Cheméo on 2024-04-26 19:36:08.358068076 +0000 UTC m=+16449417.278645387.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.