

Thiazole, 5-ethyl-2-propyl

Inchi: InChI=1S/C9H15NS/c1-3-5-9-8(10)6-7(4-2)11-9/h6H,3-5,10H2,1-2H3
InchiKey: QWCVRVGGZGKENZ-UHFFFAOYSA-N
Formula: C9H15NS
SMILES: CCCc1sc(CC)cc1N
Mol. weight [g/mol]: 169.29

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.89 | | Crippen Method |
| logp | 2.845 | | Crippen Method |
| mcvol | 144.540 | ml/mol | McGowan Method |
| rinpol | 1175.00 | | NIST Webbook |
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| rinpol | 1175.00 | | NIST Webbook |
| ripol | 1534.00 | | NIST Webbook |
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| ripol | 1534.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R61821&Units=SI>
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>

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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