

Thiazole, 4-ethyl-2-propyl-

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|-----------------------------|--|
| Other names: | 4-Ethyl-2-propylthiazole |
| Inchi: | InChI=1S/C8H13NS/c1-3-5-8-9-7(4-2)6-10-8/h6H,3-5H2,1-2H3 |
| InchiKey: | PMIYYESQWZHQKJ-UHFFFAOYSA-N |
| Formula: | C8H13NS |
| SMILES: | CCCC1nc(CC)cs1 |
| Mol. weight [g/mol]: | 155.26 |
| CAS: | 41981-68-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.02 | | Crippen Method |
| logp | 2.658 | | Crippen Method |
| mcvol | 130.450 | ml/mol | McGowan Method |
| rinpola | 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=C41981684&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpola: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/26-336-0/Thiazole-4-ethyl-2-propyl.pdf>

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