

# 4-Ethyl-1,3-thiazole

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 4-Ethylthiazole<br>Thiazole, 4-ethyl-          |
| <b>Inchi:</b>               | InChI=1S/C5H7NS/c1-2-5-3-7-4-6-5/h3-4H,2H2,1H3 |
| <b>InchiKey:</b>            | CGOVTZGCKPMLMN-UHFFFAOYSA-N                    |
| <b>Formula:</b>             | C5H7NS   |
| <b>SMILES:</b>              | CCc1cscn1                                      |
| <b>Mol. weight [g/mol]:</b> | 113.18   |
| <b>CAS:</b>                 | 17626-72-1                                     |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.80   |        | Crippen Method |
| logp          | 1.706   |        | Crippen Method |
| mcvol         | 88.180  | ml/mol | McGowan Method |
| rinpol        | 873.00  |        | NIST Webbook   |
| rinpol        | 873.00  |        | NIST Webbook   |
| rinpol        | 880.00  |        | NIST Webbook   |
| rinpol        | 873.00  |        | NIST Webbook   |
| rinpol        | 880.00  |        | NIST Webbook   |
| rinpol        | 916.00  |        | NIST Webbook   |
| ripol         | 1281.00 |        | NIST Webbook   |
| ripol         | 1281.00 |        | NIST Webbook   |
| ripol         | 1281.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626721&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626721&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |

# Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>ripol:</b>   | Polar retention indices             |

Latest version available from:

<https://www.cheméo.com/cid/80-820-2/4-Ethyl-1-3-thiazole.pdf>

Generated by Cheméo on 2024-04-24 22:07:07.367037216 +0000 UTC m=+16285676.287614528.

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