

# 1,3,4-Thiadiazole-2(3H)-thione, 5-amino-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2-Amino-5-mercapto-1,3,4-thiadiazole<br>5-Amino-2-mercapto-1,3,4-thiadiazole<br>2-Amino-1,3,4-thiadiazole-5-mercaptan<br>2-Amino-1,3,4-thiadiazole-5-thiol<br>5-Amino-1,3,4-thiadiazole-2-thiol<br>2-Amino-«delta»2-1,3,4-thiadiazoline-5-thione<br>5-Amino-1,3,4-thiadiazoline-2-thione<br>2-Mercapto-5-amino-1,3,4-thiadiazole<br>1,3,4-Thiadiazole-2-thiol, 5-amino-<br>«DELTA»2-1,3,4-Thiadiazoline-2-thiol, 5-imino-<br>2-Thiol-5-amino-1,3,4-thiadiazole<br>2-Amino-5-mercaptothiadiazole<br>USAF PD-25<br>NSC 21402<br>5-Amino-1,3,4-thiadiazole-2(3H)-thione<br>5-Thiol-2-amino-1,3,4-thiadiazole<br>NSC 209061 |
| <b>Inchi:</b>               | InChI=1S/C2H3N3S2/c3-1-4-5-2(6)7-1/h(H2,3,4)(H,5,6)   |
| <b>InchiKey:</b>            | GDGIVSREGUOIJZ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C2H3N3S2  |
| <b>SMILES:</b>              | Nc1nnc(S)s1   |
| <b>Mol. weight [g/mol]:</b> | 133.19  |
| <b>CAS:</b>                 | 2349-67-9   |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | -0.91  |        | Crippen Method |
| logp          | 0.409  |        | Crippen Method |
| mcvol         | 82.220 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <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> |

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2349679&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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