

# 1H-Tetrazole-1,5-diamine

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 1,5-Diaminotetrazol<br>1,5-diamino-tetrazolium  |
| <b>Inchi:</b>               | InChI=1S/CH4N6/c2-1-4-5-6-7(1)3/h3H2,(H2,2,4,6) |
| <b>InchiKey:</b>            | XMGWNAIPGOPSNX-UHFFFAOYSA-N                     |
| <b>Formula:</b>             | CH5CIN6O4                                       |
| <b>SMILES:</b>              | Nc1nnnn1N                                       |
| <b>Mol. weight [g/mol]:</b> | 200.54  |
| <b>CAS:</b>                 | 2165-21-1                                       |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | 0.51   |        | Crippen Method |
| logp          | -2.031 |        | Crippen Method |
| mcvol         | 65.370 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2165211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2165211&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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     |

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