

# 1-Methylhexahydropyrimidine

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C5H12N2/c1-7-4-2-3-6-5-7/h6H,2-5H2,1H3 |
| <b>InchiKey:</b>            | AHEKENQPEQYCMG-UHFFFAOYSA-N                     |
| <b>Formula:</b>             | C5H12N2   |
| <b>SMILES:</b>              | CN1CCCNC1                                       |
| <b>Mol. weight [g/mol]:</b> | 100.16  |
| <b>CAS:</b>                 | 31952-00-8                                      |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | -0.06  |        | Crippen Method |
| logp          | -0.131 |        | Crippen Method |
| mcvol         | 90.410 | 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>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C31952008&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31952008&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>                                     |

## 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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