

# 1H-Imidazole-4-ethanamine, N,N-dimethyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | N,N-Dimethylhistamine<br>Imidazole, 4-[2-(dimethylamino)ethyl]-<br>N«alpha»,N«alpha»-Dimethylhistamine<br>N«omega»,N«omega»-Dimethylhistamine<br>N',N'-Dimethylhistamine<br>4-(2-Dimethylaminoethyl)imidazole<br>N-alpha,N-alpha-Dimethylhistamine<br>N-omega,N-omega-Dimethylhistamine<br>SU-416 |
| <b>Inchi:</b>               | InChI=1S/C7H13N3/c1-10(2)4-3-7-5-8-6-9-7/h5-6H,3-4H2,1-2H3,(H,8,9)  |
| <b>InchiKey:</b>            | ZJDIMSMQXMWMCF-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H13N3   |
| <b>SMILES:</b>              | CN(C)CCc1c[nH]cn1   |
| <b>Mol. weight [g/mol]:</b> | 139.20  |
| <b>CAS:</b>                 | 673-46-1  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| affp          | 1022.00 | kJ/mol | NIST Webbook   |
| basg          | 990.10  | kJ/mol | NIST Webbook   |
| log10ws       | -0.67   |        | Crippen Method |
| logp          | 0.032   |        | Crippen Method |
| mcvol         | 119.970 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C673461&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C673461&amp;Units=SI</a> |

# Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>affp:</b>    | Proton affinity                     |
| <b>basg:</b>    | Gas basicity                        |
| <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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