

Histamine

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|-----------------------------|---|
| Other names: | 1H-Imidazole-4-ethanamine «beta»-Imidazolyl-4-ethylamine Eramin Ergamine Ergotidine Imidazole-4-ethylamine 2-(4-Imidazolyl)ethylamine 5-Imidazoleethylamine Ethylamine, 2-imidazol-4-yl- Free histamine Imidazole, 4-(2-aminoethyl)- Theramine 4-(2-Aminoethyl)-1H-imidazole «beta»-Aminoethylglyoxaline «beta»-Aminoethylimidazole NSC 33792 2-imidazol-4-ylethylamine |
| Inchi: | InChI=1S/C5H9N3/c6-2-1-5-3-7-4-8-5/h3-4H,1-2,6H2,(H,7,8) |
| InchiKey: | NTYJJOPFIAHURM-UHFFFAOYSA-N |
| Formula: | C5H9N3 |
| SMILES: | NCCc1cnc[nH]1 |
| Mol. weight [g/mol]: | 111.15 |
| CAS: | 51-45-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| affp | 999.80 | kJ/mol | NIST Webbook |
| basg | 961.90 | kJ/mol | NIST Webbook |
| log10ws | -0.69 | | Crippen Method |
| logp | -0.571 | | Crippen Method |
| mcvol | 91.790 | ml/mol | McGowan Method |
| rinpol | 1500.00 | | NIST Webbook |
| rinpol | 1497.00 | | NIST Webbook |
| rinpol | 1497.00 | | NIST Webbook |
| rinpol | 1500.00 | | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 440.20 | K | 0.10 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C51456&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|-------------------------------------|
| affp: | Proton affinity |
| basg: | Gas basicity |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpola: | Non-polar retention indices |
| tbrp: | Boiling point at reduced pressure |

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<https://www.chemeo.com/cid/88-044-6/Histamine.pdf>

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