

Ethanol, 2-[(n-methyl-n-purin-2-yl)amino]-

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C8H11N5O/c1-13(2-3-14)8-9-4-6-7(12-8)11-5-10-6/h4-5,14H,2-3H2,1H3,(H,9,10) |
| InchiKey: | PEPIMBKCCHEOGN-UHFFFAOYSA-N |
| Formula: | C8H11N5O |
| SMILES: | CN(CCO)c1ncc2[nH]cnc2n1 |
| Mol. weight [g/mol]: | 193.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.38 | | Crippen Method |
| logp | -0.700 | | Crippen Method |
| mcvol | 140.430 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008231&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/14-100-4/Ethanol-2-n-methyl-n-purin-2-yl-amino.pdf>

Generated by Cheméo on 2024-05-02 20:44:31.937600425 +0000 UTC m=+16971920.858177736.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.