

1,2-dimethyl-3-hydroxypyridin-4-one

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|----------------------|---|
| Other names: | 3-hydroxy-1,2-dimethylpyridin-4(1H)-one deferiprone |
| Inchi: | InChI=1S/C7H9NO2/c1-5-7(10)6(9)3-4-8(5)2/h3-4,10H,1-2H3 |
| InchiKey: | TZXKOCQBRNJULO-UHFFFAOYSA-N |
| Formula: | C7H9NO2 |
| SMILES: | Cc1c(O)c(=O)ccn1C |
| Mol. weight [g/mol]: | 139.15 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|---|
| hfus | 32.10 | kJ/mol | Thermodynamic Modeling and Solubility Measurement of Cetirizine Hydrochloride and Deferiprone in Pure Solvents of Acetonitrile, Ethanol, Acetic Acid, Sulfolane, and Ethyl Acetate and Their Mixtures |
| log10ws | -2.21 | | Crippen Method |
| logp | 0.399 | | Crippen Method |
| mcvol | 107.450 | ml/mol | McGowan Method |
| tt | 554.05 | K | Thermodynamic Modeling and Solubility Measurement of Cetirizine Hydrochloride and Deferiprone in Pure Solvents of Acetonitrile, Ethanol, Acetic Acid, Sulfolane, and Ethyl Acetate and Their Mixtures |

Sources

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| Thermodynamic Modeling and Solubility Measurement of Cetirizine Hydrochloride and Deferiprone in Pure Solvents of Acetonitrile, Ethanol, Acetic Acid, Sulfolane, and Ethyl Acetate and Their Mixtures: | https://www.doi.org/10.1021/acs.jced.9b00620 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| hfus: | Enthalpy of fusion at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tt: | Triple Point Temperature |

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