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

Other names: 3-hydroxy-1,2-dimethylpyridin-4(1H)-one

deferiprone

InChl=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	К	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

Thermodynamic Modeling and Solubility Measurement of Cetirizine McGowalo Mediardi Deferiprone in Pure Solvents of Acetonitrile, Ethanol, Acetone Acid; Sulfolane, and Ethyl Acetote Method: Mixtures:

https://www.doi.org/10.1021/acs.jced.9b00620 http://link.springer.com/article/10.1007/BF02311772 http://pubs.acs.org/doi/abs/10.1021/ci990307l https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficientmcvol: McGowan's characteristic volume

tt: Triple Point Temperature

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