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

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

Legend

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