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

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

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