2-nitropyridin-3-ol

Other names: 3-hydroxy-2-nitropyridine

InChl=1S/C5H4N2O3/c8-4-2-1-3-6-5(4)7(9)10/h1-3,8H

InchiKey: QBPDSKPWYWIHGA-UHFFFAOYSA-N

Formula: C5H4N2O3

SMILES: O=[N+]([O-])c1ncccc1O

Mol. weight [g/mol]: 140.10

Physical Properties

Property code	Value	Unit	Source
hfus	22.04	kJ/mol	Solubility Measurement and Modeling of 3-Hydroxy-2-nitropyridine in Ten Pure Solvents and Two Binary Mixed Solvents for T = (278.15-318.15) K
log10ws	-1.44		Crippen Method
logp	0.695		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
tt	342.77	К	Solubility Measurement and Modeling of 3-Hydroxy-2-nitropyridine in Ten Pure Solvents and Two Binary Mixed Solvents for T = (278.15-318.15) K

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Solubility Measurement and Modeling of 3-Hydroxy-2-nitropyridine in Ten MacConverted and Two Binary Mixed Solvents for T = (278.15-318.15) K:

https://www.doi.org/10.1021/acs.jced.9b00564

http://link.springer.com/article/10.1007/BF02311772

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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