

3-Nitropyridine

Inchi: InChI=1S/C5H4N2O2/c8-7(9)5-2-1-3-6-4-5/h1-4H
InchiKey: QLILRKBRWXALIE-UHFFFAOYSA-N
Formula: C5H4N2O2
SMILES: O=[N+]([O-])c1cccnc1
Mol. weight [g/mol]: 124.10
CAS: 2530-26-9

Physical Properties

Property code	Value	Unit	Source
ie	10.30 ± 0.10	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	0.990		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
tb	489.20	K	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2530269&Units=SI&Mask=3FFF>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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