

3-chloro-pyridine-1-oxide

Inchi: InChI=1S/C5H4ClNO/c6-5-2-1-3-7(8)4-5/h1-4H
InchiKey: NEXUNCTUUDERGR-UHFFFAOYSA-N
Formula: C5H4ClNO
SMILES: [O-][n+]1cccc(Cl)c1
Mol. weight [g/mol]: 129.54
CAS: 1851-22-5

Physical Properties

Property code	Value	Unit	Source
affp	902.20	kJ/mol	NIST Webbook
basg	869.70	kJ/mol	NIST Webbook
log10ws	-3.68		Crippen Method
logp	0.973		Crippen Method
mcvol	85.640	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1851225&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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