

2,6-Lutidine-N-oxide

Other names:	1-Oxide-2,6-lutidine 2,6-Dimethylpyridine N-oxide 2,6-Dimethylpyridine oxide 2,6-Dimethylpyridine-1-oxide 2,6-Dimethylpyridinium N-oxide 2,6-Lutidine oxide 2,6-Lutidine-1-oxide 2,6-dimethylpyridine-N-oxide 2,6-lutadine, 1-oxide- IVIN NSC 18258 NSC 60738 Pyridine, 2,6-dimethyl-, 1-oxide
Inchi:	InChI=1S/C7H9NO/c1-6-4-3-5-7(2)8(6)9/h3-5H,1-2H3
InchiKey:	LIDGFHXPUOJZMK-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	<chem>Cc1cccc(C)[n+]1[O-]</chem>
Mol. weight [g/mol]:	123.15
CAS:	1073-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	0.937		Crippen Method
mcvol	101.580	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Toward an inherently safer alternative for operating N-oxidation of 2,6-lutidine	https://www.doi.org/10.1016/j.tca.2017.08.007
McGowan Method	http://link.springer.com/article/10.1007/BF02311772
Effect of N-oxide on lutidine - water phase separation:	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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