2,6-LUTIDINE 1-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-
	2,6-lutidine-N-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:	Cc1cccc(C)[n+]1[O-]
Mol. weight [g/mol]:	123.15

Physical Properties

Property code	Value	Unit	Source
hf	83.48	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
logp	0.937		Crippen Method
mcvol	101.580	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Toward an inherently safer alternative for operating N-oxidation of alkylpyridines: https://www.doi.org/10.1016/j.tca.2017.08.007

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073230&Units=SI

Effect of N-oxide on lutidine - water phase separation:

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

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume