4-(N-Nitroso-N-methylamino)-1-(3-pyridyl)-1-butar

Other names:	NNK
	4-(N-Methyl-N-nitrosamino)-1-(3-pyridyl)-1-butanone
	1-Butanone, 4-(N-methyl-N-nitrosamino)-1-(3-pyridyl)
	Ketone, 3-pyridyl 3-(N-methyl-N-nitrosamino)propyl
	4-(Methyl-N-nitrosamino)-1-(3-pyridyl)-1-butanone
	N-Methyl-N-nitroso-4-oxo-4-(3-pyridyl)butyl amine
Inchi:	InChI=1S/C10H13N3O2/c1-13(12-15)7-3-5-10(14)9-4-2-6-11-8-9/h2,4,6,8H,3,5,7H2,1H3
InchiKey:	FLAQQSHRLBFIEZ-UHFFFAOYSA-N
Formula:	C10H13N3O2
SMILES:	CN(CCCC(=O)c1cccnc1)N=O
Mol. weight [g/mol]:	207.23
CAS:	64091-91-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	1.658		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64091914&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices