

Morpholine, 4-(5-nitro-2-pyridyl)-

Inchi:	InChI=1S/C9H11N3O3/c13-12(14)8-1-2-9(10-7-8)11-3-5-15-6-4-11/h1-2,7H,3-6H2
InchiKey:	FYJXIPHXFGFEGT-UHFFFAOYSA-N
Formula:	C9H11N3O3
SMILES:	O=[N+]([O-])c1ccc(N2CCOCC2)nc1
Mol. weight [g/mol]:	209.20
CAS:	26820-62-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	0.826		Crippen Method
mcvol	146.300	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26820622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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<https://www.chemeo.com/cid/12-442-7/Morpholine-4-5-nitro-2-pyridyl.pdf>

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