2-(p-Nitrobenzyl)pyridine

Other names:	Pyridine, 2-(p-nitrobenzyl)-
	Pyridine, 2-((4-nitrophenyl)methyl)-
	2-(4-Nitrobenzyl)pyridine
	Pyridine, 2-(4-nitrobenzyl)-
Inchi:	InChI=1S/C12H10N2O2/c15-14(16)12-6-4-10(5-7-12)9-11-3-1-2-8-13-11/h1-8H,9H2
InchiKey:	YBRDBYGCEIDLBX-UHFFFAOYSA-N
Formula:	C12H10N2O2
SMILES:	O=[N+]([O-])c1ccc(Cc2ccccn2)cc1
Mol. weight [g/mol]:	214.22
CAS:	620-87-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.581		Crippen Method
mcvol	159.820	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=C620871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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