

Pyridine, 4-[(4-nitrophenyl)methyl]-

Other names:	Pyridine, 4-(p-nitrobenzyl)- «gamma»-(p-Nitrobenzyl)pyridine «gamma»-(4-Nitrobenzyl)pyridine 4-(p-Nitrobenzyl)pyridine 4-(4-Nitrobenzyl)pyridine 1-(p-Nitrobenzyl)pyridine 4-(4'-Nitrobenzyl)pyridine NSC 83591
Inchi:	InChI=1S/C12H10N2O2/c15-14(16)12-3-1-10(2-4-12)9-11-5-7-13-8-6-11/h1-8H,9H2
InchiKey:	MNHKUCBXXMFQDM-UHFFFAOYSA-N
Formula:	C12H10N2O2
SMILES:	O=[N+]([O-])c1ccc(Cc2ccncc2)cc1
Mol. weight [g/mol]:	214.22
CAS:	1083-48-3

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1083483&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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