

2-(Benzylamino)-5-nitropyridine

Inchi:	InChI=1S/C12H11N3O2/c16-15(17)11-6-7-12(14-9-11)13-8-10-4-2-1-3-5-10/h1-7,9H,8H2
InchiKey:	DPOYSZDFYVXWFW-UHFFFAOYSA-N
Formula:	C12H11N3O2
SMILES:	O=[N+]([O-])c1ccc(NCc2ccccc2)nc1
Mol. weight [g/mol]:	229.23
CAS:	21626-41-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.602		Crippen Method
mcvol	169.800	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21626415&Units=SI

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/27-626-7/2-Benzylamino-5-nitropyridine.pdf>

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