

Pyridine, 4-benzyl-

Other names:	Pyridine, 4-(phenylmethyl)- «gamma»-Benzylpyridine Ba 33216 4-Benzylpyridine
Inchi:	InChI=1S/C12H11N/c1-2-4-11(5-3-1)10-12-6-8-13-9-7-12/h1-9H,10H2
InchiKey:	DBOLXXRVIFGDTI-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	<chem>c1ccc(Cc2ccncc2)cc1</chem>
Mol. weight [g/mol]:	169.22
CAS:	2116-65-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.672		Crippen Method
mcvol	142.400	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2116656&Units=SI
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

Legend

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

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