

Pyridine, 2-(2-phenylethyl)-

Other names:	Pyridine, 2-phenethyl- 2-(2-Phenylethyl)pyridine 2-Phenethylpyridine 2-Picoline, «alpha»-benzyl-
Inchi:	InChI=1S/C13H13N/c1-2-6-12(7-3-1)9-10-13-8-4-5-11-14-13/h1-8,11H,9-10H2
InchiKey:	NIJWAAUHTPDGOM-UHFFFAOYSA-N
Formula:	C13H13N
SMILES:	<chem>c1ccc(CCc2ccccc2)cc1</chem>
Mol. weight [g/mol]:	183.25
CAS:	2116-62-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.867		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
rinsol	1531.00		NIST Webbook

Sources

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=C2116623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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