

bis-(2-Picolyl)amine

Other names:	N-(2-pyridylmethyl)pyridine-2-methylamine
Inchi:	InChI=1S/C12H13N3/c1-3-7-14-11(5-1)9-13-10-12-6-2-4-8-15-12/h1-8,13H,9-10H2
InchiKey:	KXZQYLBVMZGIKC-UHFFFAOYSA-N
Formula:	C12H13N3
SMILES:	<chem>c1ccc(CNCc2ccccc2)nc1</chem>
Mol. weight [g/mol]:	199.25
CAS:	1539-42-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	1.766		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
ripol	2769.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1539420&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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