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: c1ccc(CNCc2ccccn2)nc1
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