Pyridine, 4-(2-phenylethyl)-

Other names: 4-(2-Phenylethyl)pyridine
Inchi: InChI=1S/C13H13N/c1-2-4-12(5-3-1)6-7-13-8-10-14-11-9-13/h1-5,8-11H,6-7H2
InchiKey: UWLBLNRDXXHYGS-UHFFFAOYSA-N
Formula: C13H13N
SMILES: c1ccc(CCc2ccncc2)cc1
Mol. weight [g/mol]: 183.25
CAS: 2116-64-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.867		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
rinpol	1603.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2116645&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