1-(2-phenylethyl)-pyrrol

Inchi: InChI=1S/C12H13N/c1-2-6-12(7-3-1)8-11-13-9-4-5-10-13/h1-7,9-10H,8,11H2
InchiKey: KKCMGDGJMRZKJP-UHFFFAOYSA-N
Formula: C12H13N
SMILES: c1ccc(CCn2cccc2)cc1
Mol. weight [g/mol]: 171.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.731		Crippen Method
mcvol	146.700	ml/mol	McGowan Method
ripol	2085.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492712&Units=SI

Legend

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