

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(Cc2ccccc2)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/ci9903071
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

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<https://www.chemeo.com/cid/79-512-6/1-2-phenylethyl-pyrrol.pdf>

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