

1H-Indole, 5-(phenylmethoxy)-

Other names:	5-Benzyloxyindole Indole, 5-(benzyloxy)- 5-(Phenylmethoxy)-1H-indole Benzyloxy-5 indole
Inchi:	InChI=1S/C15H13NO/c1-2-4-12(5-3-1)11-17-14-6-7-15-13(10-14)8-9-16-15/h1-10,16H,1
InchiKey:	JCQLPDZCNSVBMS-UHFFFAOYSA-N
Formula:	C15H13NO
SMILES:	c1ccc(COc2ccc3[nH]ccc3c2)cc1
Mol. weight [g/mol]:	223.27
CAS:	1215-59-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	3.265		Crippen Method
mcvol	175.380	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1215594&Units=SI

Legend

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

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