

# 5-Benzyloxyindole-2-carboxylic acid

<b>Other names:</b>	1H-Indole-2-carboxylic acid, 5-(phenylmethoxy)- 5-(phenylmethoxy)-1H-indole-2-carboxylic acid
<b>Inchi:</b>	InChI=1S/C16H13NO3/c18-16(19)15-9-12-8-13(6-7-14(12)17-15)20-10-11-4-2-1-3-5-11/
<b>InchiKey:</b>	MVCLSAMNMAWXFQ-UHFFFAOYSA-N
<b>Formula:</b>	C16H13NO3
<b>SMILES:</b>	O=C(O)c1cc2cc(OCc3ccccc3)ccc2[nH]1
<b>Mol. weight [g/mol]:</b>	267.28
<b>CAS:</b>	6640-09-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	2.963		Crippen Method
mcvol	196.910	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640091&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640091&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/115-404-5/5-Benzyloxyindole-2-carboxylic-acid.pdf>

Generated by Cheméo on 2024-04-27 15:04:23.014888799 +0000 UTC m=+16519511.935466114.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.