

# N-Benzylisatoic anhydride

<b>Inchi:</b>	InChI=1S/C15H11NO3/c17-14-12-8-4-5-9-13(12)16(15(18)19-14)10-11-6-2-1-3-7-11/h1-9
<b>InchiKey:</b>	XZNZVRHSHRYPDL-UHFFFAOYSA-N
<b>Formula:</b>	C15H11NO3
<b>SMILES:</b>	O=c1oc(=O)n(Cc2ccccc2)c2ccccc12
<b>Mol. weight [g/mol]:</b>	253.25
<b>CAS:</b>	35710-05-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.41		Crippen Method
logp	2.003		Crippen Method
mcvol	182.820	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=C35710055&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35710055&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

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