

# 2(3H)- benzofuranone, 3-phenyl-3-(2-piperidinoethyl)-

<b>Inchi:</b>	InChI=1S/C21H23NO2/c23-20-21(17-9-3-1-4-10-17,13-16-22-14-7-2-8-15-22)18-11-5-6-
<b>InchiKey:</b>	QXZIRLROACDSIP-UHFFFAOYSA-N
<b>Formula:</b>	C21H23NO2
<b>SMILES:</b>	O=C1Oc2ccccc2C1(CCN1CCCCC1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	321.41
<b>CAS:</b>	116465-80-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.768		Crippen Method
mcvol	254.930	ml/mol	McGowan Method

## Sources

<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>
<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=C116465806&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116465806&amp;Units=SI</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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