

# Nicotinic acid benzyl ester

<b>Other names:</b>	3-Pyridinecarboxylic acid, phenylmethyl ester Benzyl nicotinate Benzyl pyridine-3-carboxylate Niacin benzyl ester Pyridine-3-carboxylic acid benzyl ester Rubriment Estru benzyłowego kwasu nikotynowego Pycaril Pykaryl Nicotinic acid, phenylmethyl ester
<b>Inchi:</b>	InChI=1S/C13H11NO2/c15-13(12-7-4-8-14-9-12)16-10-11-5-2-1-3-6-11/h1-9H,10H2
<b>InchiKey:</b>	KVYGGMBOZFWZBQ-UHFFFAOYSA-N
<b>Formula:</b>	C13H11NO2
<b>SMILES:</b>	O=C(OCc1ccccc1)c1cccnc1
<b>Mol. weight [g/mol]:</b>	213.23
<b>CAS:</b>	94-44-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.439		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
rmpol	1770.00		NIST Webbook
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## 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=C94440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94440&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
<b>rinpol:</b>	Non-polar retention indices

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