

# Methylphenobarbital, M(HO-), AC

<b>Inchi:</b>	InChI=1S/C15H16N2O5/c1-4-15(12(19)16-14(21)17(3)13(15)20)10-5-7-11(8-6-10)22-9(2
<b>InchiKey:</b>	OCXSXUHYEJHCKD-UHFFFAOYSA-N
<b>Formula:</b>	C15H16N2O5
<b>SMILES:</b>	CCC1(c2ccc(OC(C)=O)cc2)C(=O)NC(=O)N(C)C1=O
<b>Mol. weight [g/mol]:</b>	304.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	0.968		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
rinsol	2330.00		NIST Webbook

## Sources

<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=R255706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R255706&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinsol:</b>	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/32-582-0/Methylphenobarbital-M-HO-AC.pdf>

Generated by Cheméo on 2024-04-19 00:19:27.627950933 +0000 UTC m=+15775216.548528244.

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