

# Pentobarbital ethylated

<b>Other names:</b>	Pentobarbital, 1,3-diethyl Pentobarbital perethylated
<b>Inchi:</b>	InChI=1S/C15H26N2O3/c1-6-10-11(5)15(7-2)12(18)16(8-3)14(20)17(9-4)13(15)19/h11H
<b>InchiKey:</b>	SABMZHJKJZHPCMB-UHFFFAOYSA-N
<b>Formula:</b>	C15H26N2O3
<b>SMILES:</b>	CCCC(C)C1(CC)C(=O)N(CC)C(=O)N(CC)C1=O
<b>Mol. weight [g/mol]:</b>	282.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.650		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		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=R16282&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R16282&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/112-974-6/Pentobarbital-ethylated.pdf>

Generated by Cheméo on 2024-04-28 00:44:55.16894376 +0000 UTC m=+16554344.089521081.

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