

# 1,3-Di-n-butyl phenobarbital

<b>Other names:</b>	Phenobarbital perbutylated Phenobarbital butylated Phenobarbital, 1,3-dibutyl
<b>Inchi:</b>	InChI=1S/C20H28N2O3/c1-4-7-14-21-17(23)20(6-3,16-12-10-9-11-13-16)18(24)22(19(2
<b>InchiKey:</b>	MWGXCHIZNGBVJY-UHFFFAOYSA-N
<b>Formula:</b>	C20H28N2O3
<b>SMILES:</b>	CCCCN1C(=O)N(CCCC)C(=O)C(CC)(c2ccccc2)C1=O
<b>Mol. weight [g/mol]:</b>	344.45
<b>CAS:</b>	73897-12-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	3.725		Crippen Method
mcvol	282.710	ml/mol	McGowan Method
rinpol	2238.00		NIST Webbook
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook
rinpol	2261.00		NIST Webbook
rinpol	2238.00		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=C73897128&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C73897128&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

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/125-285-7/1-3-Di-n-butyl-phenobarbital.pdf>

Generated by Cheméo on 2024-04-30 22:07:56.782075245 +0000 UTC m=+16804125.702652560.

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