

1-N-butyl-phenobarbital

Inchi:	InChI=1S/C16H20N2O3/c1-3-5-11-18-14(20)16(4-2,13(19)17-15(18)21)12-9-7-6-8-10-12
InchiKey:	GZHFOXIBCWGWZSM-UHFFFAOYSA-N
Formula:	C16H20N2O3
SMILES:	CCCCN1C(=O)NC(=O)C(CC)(c2ccccc2)C1=O
Mol. weight [g/mol]:	288.34
CAS:	116495-69-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.213		Crippen Method
mcvol	226.350	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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