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: GZHFOXIBCWGZSM-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/ci990307l
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