1,3-Di-n-butyl phenobarbital

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C73897128&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

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