Phenytoin di-methyl derivative

Other names:	Hydantoin, 1,3-dimethyl-5,5-diphenyl- N,N'-Dimethyldiphenylhydantoin 1,3-Dimethyl-5,5-diphenylhydantoin Dimethyl derivative of phenytoin 1,3-Dimethyl derivative of 5,5-Diphenylhydantoin Phenytoin di-methyl derivative 1,3-Dimethyl-5,5-diphenyl-2,4-imidazolidinedione Phenytoin di-Me Phenytoin, methylated Phenytoin permethylated Phenytoin Me
Inchi:	InChI=1S/C17H16N2O2/c1-18-15(20)17(19(2)16(18)21,13-9-5-3-6-10-13)14-11-7-4-8-12
InchiKey:	AQYFZMVWTWUJKL-UHFFFAOYSA-N
Formula:	C17H16N2O2
SMILES:	CN1C(=O)N(C)C(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]:	280.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Cheméo Relay (1.0)
logp	2.454		Crippen Method
mcvol	215.110	ml/mol	McGowan Method
rinpol	2213.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2264.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6456015&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices