2,4-Imidazolidinedione, 1,3-dimethyl-5,5-diphenyl-

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]:	280.32
CAS:	6456-01-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.454		Crippen Method
mcvol	215.110	ml/mol	McGowan Method
rinpol	2169.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2264.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6456015&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices