

2,4-Imidazolidinedione, 3-methyl-5,5-diphenyl-

Other names:	Hydantoin, 3-methyl-5,5-diphenyl- Hydotin Melantoin Methylphenytoin 3-Methyl-5,5-diphenylhydantoin 3-Methyl-5,5-diphenyl-2,4-imidazolidinedione
Inchi:	InChI=1S/C16H14N2O2/c1-18-14(19)16(17-15(18)20,12-8-4-2-5-9-12)13-10-6-3-7-11-13
InchiKey:	LTYDTBHSPIJPEG-UHFFFAOYSA-N
Formula:	C16H14N2O2
SMILES:	CN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]:	266.29
CAS:	4224-00-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.112		Crippen Method
mcvol	201.020	ml/mol	McGowan Method
rinpol	2299.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4224004&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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