5,5-Diphenylhydantoin, 3-acetyl-

Other names: PHENYTOIN, AC
Inchi: InChI=1S/C17H14N2O3/c1-12(20)19-15(21)17(18-16(19)22,13-8-4-2-5-9-13)14-10-6-3-7
InchiKey: KAEXLXZWCWCDPZ-UHFFFAOYSA-N
Formula: C17H14N2O3
SMILES: CC(=O)N1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.029		Crippen Method
mcvol	216.680	ml/mol	McGowan Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2444.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374835&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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