Barbituric acid, 5-methyl-5-phenyl perethylated

Inchi: InChI=1S/C15H18N2O3/c1-4-16-12(18)15(3,11-9-7-6-8-10-11)13(19)17(5-2)14(16)20/h6
InchiKey: ZYBMUAGUHQVIEA-UHFFFAOYSA-N
Formula: C15H18N2O3
SMILES: CCN1C(=O)N(CC)C(=O)C(C)(c2ccccc2)C1=O
Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.775		Crippen Method
mcvol	212.260	ml/mol	McGowan Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		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=R387769&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

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