2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3,5-trimethyl-5-phenyl-

Other names: Phenylmethylbarbituric acid-permethylated
Barbituric acid, 5-methyl-5-phenyl permethylated

Inchi: InChI=1S/C13H14N2O3/c1-13(9-7-5-4-6-8-9)10(16)14(2)12(18)15(3)11(13)17/h4-8H,1-3

InchiKey: XWUNPDJNYVBVJA-UHFFFAOYSA-N

Formula: C13H14N2O3

SMILES: CN1C(=O)N(C)C(=O)C(C)(c2ccccc2)C1=O

Mol. weight [g/mol]: 246.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	0.995		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
rinpol	1785.00		NIST Webbook
rinpol	1785.00		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=U298794&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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