Barbituric acid, 5-methyl-5-phenyl perbutylated

Inchi: InChI=1S/C19H26N2O3/c1-4-6-13-20-16(22)19(3,15-11-9-8-10-12-15)17(23)21(18(20)24
InchiKey: BDEGLSYKHQSELU-UHFFFAOYSA-N
Formula: C19H26N2O3
SMILES: CCCCN1C(=O)N(CCCC)C(=O)C(C)(c2ccccc2)C1=O
Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	3.335		Crippen Method
mcvol	268.620	ml/mol	McGowan Method
rinpol	2187.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R15735&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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