Heptabarbital monomethylated

Inchi: InChI=1S/C14H20N2O3/c1-3-14(10-8-6-4-5-7-9-10)11(17)15-13(19)16(2)12(14)18/h8H,3
InchiKey: JCJMPACNJDLUCC-UHFFFAOYSA-N
Formula: C14H20N2O3
SMILES: CCC1(C2=CCCCCC2)C(=O)NC(=O)N(C)C1=O
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	1.981		Crippen Method
mcvol	206.770	ml/mol	McGowan Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		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=R40201&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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