2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-1-ethyl-3,5-dimethyl-

Other names: Monoethylhexobarbital
N-Ethylhexobarbital
Hexobarbital ethylated
Hexobarbital perethylated

Inchi: InChI=1S/C14H20N2O3/c1-4-16-12(18)14(2,10-8-6-5-7-9-10)11(17)15(3)13(16)19/h8H,4

InchiKey: IAXQVVJGNSGULG-UHFFFAOYSA-N

Formula: C14H20N2O3

SMILES: CCN1C(=O)N(C)C(=O)C(C)(C2=CCCCC2)C1=O

Mol. weight [g/mol]: 264.32

CAS: 55044-42-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	1.934		Crippen Method
mcvol	206.770	ml/mol	McGowan Method
rinpol	1859.00		NIST Webbook
rinpol	1859.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55044423&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