

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
rinsol	1859.00		NIST Webbook
rinsol	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

Latest version available from:

<https://www.cheméo.com/cid/120-088-1/2-4-6-1H-3H-5H-Pyrimidinetrione-5-1-cyclohexen-1-yl-1-ethyl-3-5-dimethyl.p>

Generated by Cheméo on 2024-05-01 07:05:47.465769354 +0000 UTC m=+16836396.386346666.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.