

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

Other names:

Diethylphenobarbital

N,N'-Diethylphenobarbital

1,3-Diethylphenobarbital

1,3-Diethyl derivative of phenobarbital

1,4-Diethylphenobarbital

Phenobarbital, 1,3-diethyl

Phenobarbital ethylated

Phenobarbital perethylated

Inchi:

InChI=1S/C16H20N2O3/c1-4-16(12-10-8-7-9-11-12)13(19)17(5-2)15(21)18(6-3)14(16)20

InchiKey:

UGVJFCFVDRFHFP-UHFFFAOYSA-N

Formula:

C16H20N2O3

SMILES:

CCN1C(=O)N(CC)C(=O)C(CC)(c2ccccc2)C1=O

Mol. weight [g/mol]:

288.34

CAS:

38024-60-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	2.165		Crippen Method
mcvol	226.350	ml/mol	McGowan Method
rinpol	1932.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook

## Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C38024601&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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