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 phenobarbitol
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/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