

2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-diethyl-5-(1-methylbutyl)-5-(2-propenyl)-

Other names:

Diethylsecobarbital
2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-diethyl-5-(1-methylbutyl)-5-
1,3-Diethyl derivative of secobarbital
Secobarbital, 1,3-diethyl
Secobarbital ethylated
Secobarbital perethylated

Inchi: InChI=1S/C16H26N2O3/c1-6-10-12(5)16(11-7-2)13(19)17(8-3)15(21)18(9-4)14(16)20/h7

InchiKey: OMTILYIUFEFSYGL-UHFFFAOYSA-N

Formula: C16H26N2O3

SMILES: C=CCC1(C(C)CCC)C(=O)N(CC)C(=O)N(CC)C1=O

Mol. weight [g/mol]: 294.39

CAS: 54833-76-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.816		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
rinpol	1761.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1790.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54833760&Units=SI>

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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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