

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

Other names:

Secbutarbitone-permethylated
1,3-Dimethyl derivative of butabarbital
Butobarbital-permethylated
Secbutobarbitone-permethylated
Butabarbital, 1,3-dimethyl
NSC 35505
Secbutabarbital, permethylated
Butabarbital Me

Inchi: InChI=1S/C12H20N2O3/c1-6-8(3)12(7-2)9(15)13(4)11(17)14(5)10(12)16/h8H,6-7H2,1-5H

InchiKey: GDYZVNWWINOYGP-UHFFFAOYSA-N

Formula: C₁₂H₂₀N₂O₃

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

Mol. weight [g/mol]: 240.30

CAS: 55134-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	1.479		Crippen Method
mcvol	193.750	ml/mol	McGowan Method
rinpol	1557.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1545.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55134037&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
rinpolar:	Non-polar retention indices

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