Barbituric acid, 5,5-diallyl-1,3-dimethyl-

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl-5,5-di-2-propenyl-
	Dimethylallobarbital
	N,N-Dimethylallobarbitone
	5,5-Diallyl-1,3-dimethylbarbituric acid
	Dimethyldial
	1,3-Dimethyl derivative of allobarbitol
	Dimethylallobarbitone
	Allobarbitone-permethylated
	5,5-Diallyl-1,3-dimethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	Allobarbital permethylated
	NSC 125779
Inchi:	InChI=1S/C12H16N2O3/c1-5-7-12(8-6-2)9(15)13(3)11(17)14(4)10(12)16/h5-6H,1-2,7-8H
InchiKey:	MCTNRBUJWLUDJG-UHFFFAOYSA-N
Formula:	C12H16N2O3
SMILES:	C=CCC1(CC=C)C(=O)N(C)C(=O)N(C)C1=O
Mol. weight [g/mol]:	236.27
CAS:	722-97-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Crippen Method
logp	1.175		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1491.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C722974&Units=SI

Legend

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