Methohexital

Other names:	Methohexitone
	Barbituric acid, 5-allyl-1-methyl-5-(1-methyl-2-pentynyl)-, (.+/-.)-
	Barbituric acid, 5-allyl-1-methyl-5-(1-methyl-2-pentynyl)-
	Brevital
	Brietal
	Methodrexitone
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 1-methyl-5-(1-methyl-2-pentynyl)-5-(2-propenyl)-, (.+/-.)-
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 1-methyl-5-(1-methyl-2-pentynyl)-5-(2-propenyl)-
	5-Allyl-1-methyl-5-(1-methyl-2-pentynyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	Enallynymall
	5-Allyl-5-(3-hexyn-2-yl)-1-methylbarbituric acid
	Compound 22451
	Compound 25398
Inchi:	InChI=1S/C14H18N2O3/c1-5-7-8-10(3)14(9-6-2)11(17)15-13(19)16(4)12(14)18/h6,10H,2
InchiKey:	NZXKDOXHBHYTKP-UHFFFAOYSA-N
Formula:	C14H18N2O3
SMILES:	C=CCC1(C(C)C#CCC)C(=O)NC(=O)N(C)C1=O
Mol. weight [g/mol]:	262.30
CAS:	151-83-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.307		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
rinpol	1770.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tf	365.00 ± 1.00	K	NIST Webbook

Sources

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=C151837&Units=SI

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point