2,4,6(1H,3H,5H)-Pyrimidinetrione, 1-methyl-5-(1-methylethyl)-5-(2-propenyl)-

Other names: Barbituric acid, 5-allyl-5-isopropyl-1-methyl-
Enallylpropymal
Narconumal
1-Methyl-5-(1-methylethyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-allyl-5-isopropyl-1-methylbarbituric acid

Inchi: InChI=1S/C11H16N2O3/c1-5-6-11(7(2)3)8(14)12-10(16)13(4)9(11)15/h5,7H,1,6H2,2-4H3

InchiKey: AXJXURWWUFZZKN-UHFFFAOYSA-N

Formula: C11H16N2O3

SMILES: C=CCC1(C(C)C)C(=O)NC(=O)N(C)C1=O

Mol. weight [g/mol]: 224.26

CAS: 1861-21-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	0.913		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
rinpol	1561.00		NIST Webbook
tf	329.50 ± 0.50	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.00 ± 1.00	K	1.60	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1861218&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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point