Tetrabenazine

Other names:	2H-Benzo[a]quinolizin-2-one, 1,3,4,6,7,11b-hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-
	Nitoman
	Ro 1-9569
	Ro 1-9569/12
	Rubigen
	Tetrabenazin
	Tetrabenzaine
	Tetrabenzine
	1,3,4,6,7,11b-Hexahydro-3-isobutyl-9,10-dimethoxy-2H-benzo(a)quinolizin-2-one
	2-Oxo-3-isobutyl-9,10-dimethoxy-1,2,3,4,6,7,11b-hexahydro-2H-benzo(a)quinolizine
	2H-Benzo(a)quinolizin-2-one, 1,3,4,6,7,11b-hexahydro-3-isobutyl-9,10-dimethoxy-
	1,2,4,6,7,11b-Hexahydro-3-isobutyl-9,10-dimethoxy-2H-benzo[a]quinolizin-2-one
	NSC 169886
Inchi:	InChI=1S/C19H27NO3/c1-12(2)7-14-11-20-6-5-13-8-18(22-3)19(23-4)9-15(13)16(20)10-1
InchiKey:	MKJIEFSOBYUXJB-UHFFFAOYSA-N
Formula:	C19H27NO3
SMILES:	COc1cc2c(cc1OC)C1CC(=O)C(CC(C)C)CN1CC2
Mol. weight [g/mol]:	317.42
CAS:	58-46-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	3.238		Crippen Method
mcvol	256.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58468&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume