Tazettine

Other names:	Sekisanin Sekisanolin Sekisanoline Tazetine Tazettin Ungernin Ungernine 8H-[1,3]Dioxolo[6,7][2]benzopyrano[3,4-c]indol-6a(3H)-ol, 4,4a,5,6-tetrahydro-3-methoxy-5-methyl-, (3S,4aS,6aS,13bS)- 8H-[1,3]Dioxolo[6,7][2]benzopyrano[3,4-c]indol-6a(3H)-ol, 4,4a,5,6-tetrahydro-3-methoxy-5-methyl-, [3S-(3«alpha»,4a«alpha»,6a«beta»,13bR*)]- Sekisanine [3S-(3«alpha»,4a«alpha»,6a«beta»,13bR*)]-4,4a,5,6-Tetrahydro-3-methoxy-5-methyl-8H- NSC 115495 NSC 652297
Inchi:	InChI=1S/C18H21NO5/c1-19-9-18(20)17(4-3-12(21-2)6-16(17)19)13-7-15-14(22-10-23-1
InchiKey:	YLWAQARRNQVEHD-UHFFFAOYSA-N
Formula:	C18H21NO5
SMILES:	COC1C=CC23c4cc5c(cc4COC2(O)CN(C)C3C1)OCO5
Mol. weight [g/mol]:	331.36
CAS:	507-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	1.161		Crippen Method
mcvol	232.310	ml/mol	McGowan Method
rinpol	2590.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507799&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