

# 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-,

Sekisanin

[3S-(3«alpha»,4a«alpha»,6a«beta»,13bR\*)]-

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(22-10-23-11)**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
rinpola	2590.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>**Crippen Method:** [https://www.chemed.com/doc/models/crippen\\_log10ws](https://www.chemed.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=C507799&Units=SI>

# Legend

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

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