# Gelsemine

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|---|---|
| **Other names:** | Spiro[3,5,8-ethanylylidene-1H-pyrano[3,4-c]pyridine-10,3'-[3H]indol]-2'(1'H)-one, 5-ethenyl-3,4,4a,5,6,7,8,8a-octahydro-7-methyl-, [3R-(3«alpha»,4a«beta»,5«alpha»,8«alpha»,8a«beta»,9S*,10S*)]-<br>Spiro[3,5,8-ethanylylidene-1H-pyrano[3,4-c]pyridine-10,3'-[3H]indol]-2'(1'H)-one, 5-ethenyl-3,4,4a,5,6,7,8,8a-octahydro-7-methyl-, gelsemin<br>Spiro[3,5,8-ethanylylidene-1H-pyrano[3,4-c]pyridine-10,3'-[3H]indole] , gelsemine deriv.<br>[3R-(3«alpha»,4a«beta»,5«alpha»,8«alpha»,8a«beta»,9S*,10S*)]-5-Etheny l-3,4,4a,5,6,7,8,8a-octahydro-7-methylspiro[3,5,8-ethanylylidene-1H-p yrano[3,4-c]pyridine-10,3'-[3H]indol]-2'(1'H)-one |
| **Inchi:** | Spiro[3,5,8-ethanylylidene-1H-pyrano[3,4-c]pyridine-10,3'-[3H]indol]-2'(1'H)-one, 5-ethenyl-3,4,4a,5,6,7,8,8a-octahydro-7-methyl-, [3R-(3«alpha»,4a«beta»,5«alpha»,8«alpha»,8a«beta»,9S,10S)]-<br>InChI=1S/C20H22N2O2/c1-3-19-10-22(2)16-11-9-24-15(8-13(11)19)20(17(16)19)12-6-4- |
| **InchiKey:** | NFYYATWFXNPTRM-UHFFFAOYSA-N |
| **Formula:** | C20H22N2O2 |
| **SMILES:** | C=CC12CN(C)C3C4COC(CC41)C1(C(O)=Nc4ccccc41)C32 |
| **Mol. weight [g/mol]:** | 322.40 |
| **CAS:** | 509-15-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.76 | | Crippen Method |
| logp | 2.677 | | Crippen Method |
| mcvol | 237.700 | ml/mol | McGowan Method |

# Sources

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| **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=C509159&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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