

# Spiro[2,5-cyclohexadiene-1,7'(1'H)-cyclopent[ij]isoxan-2,3,8,8'a-tetrahydro-5',6'-dimethoxy-1'-methyl-, (R)-

Other names:

Pronuciferine

Milthanthine

Pronuciferin

N-Methylstepharine

N,O-Dimethylcrotonosine

(+)-Pronuciferine

**Inchi:** InChI=1S/C19H21NO3/c1-20-9-6-12-10-15(22-2)18(23-3)17-16(12)14(20)11-19(17)7-4-1

**InchiKey:** WUYQEGNOQLRQAQ-CQSZACIVSA-N

**Formula:** C19H21NO3

**SMILES:** COc1cc2c3c(c1OC)C1(C=CC(=O)C=C1)CC3N(C)CC2

**Mol. weight [g/mol]:** 311.37

**CAS:** 2128-60-1

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.59   |        | Crippen Method |
| logp          | 2.569   |        | Crippen Method |
| mcvol         | 236.920 | ml/mol | McGowan Method |
| rinpol        | 2676.00 |        | NIST Webbook   |
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## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C2128601&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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