

# Pyrrolidine, 1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]- (E,E)-

Other names:

Pyrrolidine, 1-piperoyl-, (E,E)-

Piperylin

Piperyline

Trichostachin

Trichostachine

5-(Methylenedioxyphenyl)-2,4-pentadienoyl pyrrolidide (Piperylin)

(2E,4E)-5-(Benzo[d][1,3]dioxol-5-yl)-1-(pyrrolidin-1-yl)penta-2,4-dien-1-one

**Inchi:** InChI=1S/C16H17NO3/c18-16(17-9-3-4-10-17)6-2-1-5-13-7-8-14-15(11-13)20-12-19-14/

**InchiKey:** GQIJYUMTOUBHSH-IJIVKGSJSA-N

**Formula:** C16H17NO3

**SMILES:** O=C(C=CC=Cc1ccc2c(c1)OCO2)N1CCCC1

**Mol. weight [g/mol]:** 271.31

**CAS:** 25924-78-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	2.607		Crippen Method
mcvol	205.510	ml/mol	McGowan Method
rinpol	2892.60		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	2892.60		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C25924781&Units=SI>

**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>

# 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>rinpola:</b>	Non-polar retention indices

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