

# Spiro[2H-1-benzopyran-2,2'-[2H]indole], 1',3'-dihydro-1',3',3'-trimethyl-6-nitro-

Other names:

Spiro[2H-1-benzopyran-2,2'-indoline], 1',3',3'-trimethyl-6-nitro-

1',3',3'-Trimethyl-6-nitrospiro[2H-1-benzopyran-2,2'-indoline]

6'-Nitro-1,3,3-trimethylindolinobenzopyrylspiran

1,3,3-Trimethylindolino-6'-nitrobenzopyrylospiran

Spiro(2H-1-benzopyran-2,2'-indoline), 6-nitro-1',3',3'-trimethyl-

1,3,3-Trimethyl-6'-nitroindoline-2-spiro-2'-benzopyran

1',3'-dihydro-1',3',3'-trimethyl-6-nitrospiro[2H-1-benzopyran-2,2'-[2H]indole]

1',3',3'-Trimethyl-6-nitro-spiro[2-(2H-benzopyran)-2'-indolenine]

Inchi:

InChI=1S/C19H18N2O3/c1-18(2)15-6-4-5-7-16(15)20(3)19(18)11-10-13-12-14(21(22)23)

InchiKey:

PSXPTGAEJZYNFI-UHFFFAOYSA-N

Formula:

C19H18N2O3

SMILES:

CN1c2ccccc2C(C)(C)C12C=Cc1cc([N+](=O)[O-])ccc1O2

Mol. weight [g/mol]:

322.36

CAS:

1498-88-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	4.124		Crippen Method
mcvol	238.300	ml/mol	McGowan Method

## 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=C1498880&Units=SI>

## Legend

log10ws:

Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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