

# Griseofulvin

## Other names:

(+)-Griseofulvin

(1'S,6'R)-7-chloro-2',4,6-trimethoxy-6'-methyl-3H-spiro[benzofuran-2,1'-cyclohex[2]ene]-3

([1S],trans-7-chloro-2',4,6-trimethoxy-6'-methylspiro[benzofuran-2(3H),1'-(2)cyclohexene]-3,4  
(7-Chloro-2',4,6-trimethoxy-6' «beta»-methylspiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4  
(griseofulvin)

7-Chloro-2',4,6-trimethoxy-6'Â«betaÂ»-methylspiro[benzofuran-2(3H),1'-[2]cyclohexene]-

7-Chloro-4,6,2'-trimethoxy-6'-methylgris-2'-en-3,4'-dione

Amudane

Biogrisin-FP

Curling factor

Delmofulvina

Fulcin

Fulcine

Fulvican grisactin

Fulvicin

Fulvicin Bolus

Fulvicin-P/G

Fulvicin-U/F

Fulvina

Fulvinil

Fulvistatin

Fungivin

Greosin

Gresfeed

Gricin

Grifulin

Grifulvin

Grifulvin V

Gris-PEG

Grisactin

Griscofulvin

Grisefuline

Griseo

Griseofulvin, (+)-

Griseofulvin-forte

Griseofulvinum

Grisetin

Grisofulvin

Grisovin

Grisovin FP

Grizeofulvin

Gryso  
 Guservin  
 Lamoryl  
 Likuden  
 Likunden  
 Murfulvin  
 NSC 34533  
 Neo-Fulcin  
 Polygris  
 Poncyl  
 Spiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione,  
 7-chloro-2',4,6-trimethoxy-6'-methyl-, (1'S,6'R)-  
 Spiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione,  
 7-chloro-2',4,6-trimethoxy-6'-methyl-, (1'S-trans)-  
 Spiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione,  
 7-chloro-2',4,6-trimethoxy-6'«beta»-methyl-,  
 Spiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione,  
 7-chloro-2',4,6-trimethoxy-6'«beta»-methyl-,  
 Spirofulvin  
 Sporostatin  
 Sporostatin xan  
 USAF SC-2  
 Xuanjing

**Inchi:** InChI=1S/C17H17ClO6/c1-8-5-9(19)6-12(23-4)17(8)16(20)13-10(21-2)7-11(22-3)14(18)1

**InchiKey:** DDUHZTYCFQRHIY-UHFFFAOYSA-N

**Formula:** C17H17ClO6

**SMILES:** COC1=CC(=O)CC(C)C12Oc1c(Cl)c(OC)cc(OC)c1C2=O

**Mol. weight [g/mol]:** 352.77

**CAS:** 126-07-8

## Physical Properties

Property code	Value	Unit	Source
gf	-379.94	kJ/mol	Joback Method
hf	-828.53	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-4.56		Aqueous Solubility Prediction Method
log10ws	-3.25		Estimated Solubility Method
logp	2.810		Crippen Method
mcvol	239.470	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2700.00		NIST Webbook

rinpol	2700.00		NIST Webbook
rinpol	2700.00		NIST Webbook
tb	928.64	K	Joback Method
tc	1178.62	K	Joback Method
tf	683.49	K	Joback Method
vc	0.899	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.41	J/mol×K	1095.29	Joback Method
cpg	829.83	J/mol×K	1136.95	Joback Method
cpg	755.85	J/mol×K	928.64	Joback Method
cpg	772.14	J/mol×K	970.30	Joback Method
cpg	787.63	J/mol×K	1011.97	Joback Method
cpg	802.36	J/mol×K	1053.63	Joback Method
cpg	842.69	J/mol×K	1178.62	Joback Method
hfust	44.70	kJ/mol	491.20	NIST Webbook
hfust	39.39	kJ/mol	495.20	NIST Webbook

## Sources

<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C126078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C126078&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Measurement and Correlation of Griseofulvin Solubility in Different Solvents at Temperatures from (281.95 to 357.60) K:</b>	<a href="https://www.doi.org/10.1021/je100030j">https://www.doi.org/10.1021/je100030j</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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