

# *AKos*

*Consulting & Solutions GmbH*



CWM Global Search – Using ChemAxon products and services in Silverlight

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Developer, AKos GmbH

ChemAxon UGM, May 17th 2011

## What is Silverlight ?

- An application framework to build Rich Internet Applications (RIA)
- Silverlight applications run in a Webbrowser on both Windows and Mac
- It is a Microsoft Plug-In
- You can compare it with Adobe Flash
- Current version number is 4.0




## What is CWM Global Search ?

- A true meta search engine for free chemistry databases on the Internet
- Currently searches over up to 50 internet datasources
- One can search using structure, CAS Registry number(s) or free text (e.g. Names)
- Results are Hyperlinks

Search by name (Text may contain synonym, brand name, InChI, SMILES)

Search by CAS Registry number

Search by structure

 Double click inside box below to open structure editor  
or right click inside box below and use edit>paste to paste structure

# CWM Global Search

## The Quick Search page

CWM GlobalSearch version 4.8.5.0

QuickSearch QuickSearch Results Global Search Global Search Results

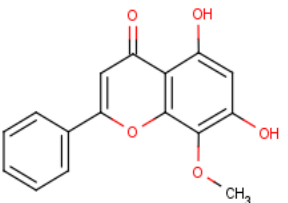
Clear Form Clear Structure Read Molfile Save Query Load Query

News | Home | Feedback | Impressum

- Search by name (Text may contain synonym, brand name, InChI, SMILES)
- Search by CAS Registry number
- Search by structure  
Double click inside box below to open structure editor  
or right click inside box below and use edit>paste to paste structure

MarvinSketch

File Edit View Insert Atom Bond Structure Tools Help



100%

H C N O S F P Cl

Tautomerize structure query? Chemical Name Search? Name to Structure? Start QuickSearch

CWM GlobalSearch version 4.8.5.0

QuickSearch | QuickSearch Results | Global Search | Global Search Results

Clear Form | Clear Structure | Read Multiple | Save Query | Load Query

News | Home | Feedback | Impressum

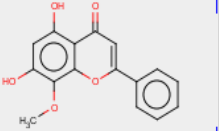
Search by name (Text)

wogonin

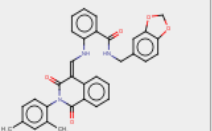
Search by CAS Register

Search by structure

Double click inside box or right click inside box



Wogonin



TS296047

Pick selected Found 2 matching structures. Cancel

Tautomerize structure query ? | Chemical Name Search ? | Name to Structure ? | Start QuickSearch

CWM GlobalSearch version 4.85.0

QuickSearch QuickSearch Results Global Search Global Search Results

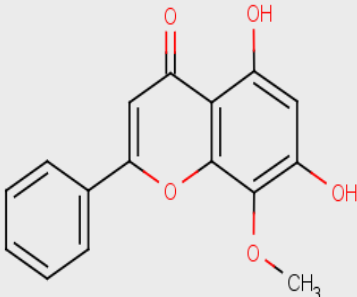
Save Result Load Result Home | Feedback | Impressum

CWMGlobalSearchQuicksearchResultsPage.xml?title=06.05.2011 21:10:02

<p>NCI IUPAC Name <span>chemicalize &gt;</span></p> <p>5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one</p> <p>ChemAxon IUPAC Name <span>chemicalize &gt;</span></p> <p>5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one</p>		<p>Names and synonyms</p> <p>4H-1-Benzopyran-4-one, 5,7-dihydroxy-8-methoxy-2-phenyl-</p> <p>5,7-Dihydroxy-8-methoxyflavone</p> <p>5-18-04-00571 (Beilstein Handbook Reference)</p> <p>AIDS001403</p> <p>AIDS-001403</p> <p>BRN 0287152</p> <p>C10197</p> <p>FLAVONE, 5,7-DIHYDROXY-8-METHOXY-</p> <p>NCI60_040649</p> <p>Norwogonin 8-methyl ether</p> <p>NSC717845</p> <p>ST077088</p> <p>Vogonin</p> <p>Wogonin</p>
<p>CAS Registry Numbers</p> <p>10-29-7</p> <p>632-85-9</p>	<p>Links</p> <p><a href="#">Thomson Pharma 00044036</a></p> <p><a href="#">NLM ChemIDplus 000632859</a></p> <p><a href="#">NIAID HIV/OI 001403</a></p> <p><a href="#">CambridgeSoft 10297</a></p> <p><a href="#">ChEMBL 117852</a></p> <p><a href="#">iResearch Library 187815833</a></p> <p><a href="#">eMolecules 2736681</a></p> <p><a href="#">iResearch Library 29543758</a></p> <p><a href="#">ChemSpider 4445020</a></p> <p><a href="#">DiscoveryGate 5281703</a></p> <p><a href="#">ChemDB 6919187</a></p> <p><a href="#">NCI Open Database 717845</a></p> <p><a href="#">KEGG C10197</a></p> <p><a href="#">ChemBank NCI60_040649</a></p>	

Select/Deselect All Copy to clipboard

Double click inside box below to view structure



Copy to clipboard Select/Deselect All

Transfer to Global Search

## The Quick Search results page – ChemAxon Chemicalize Integration

CWM GlobalSearch version 4.8.0

QuickSearch QuickSearch Results Global Search Global Search Results

Save Result Load Result

NCI IUPAC Name  
5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one

ChemAxon IUPAC Name  
5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one

CAS Registry Numbers	Links
10-29-7	Thomson Pharma 00044036
632-85-9	NLM ChemIDplus 000632859
	NIAID HIV/OI 001403
	CambridgeSoft 10297
	ChEMBL 117852
	iResearch Library 187815833
	eMolecules 2736681
	iResearch Library 29543758
	ChemSpider 4445020
	DiscoveryGate 5281703
	ChemDB 6919187
	NCI Open Database 717845
	KEGG C10197
	ChemBank NCI60_040649

Select/Deselect All Copy to clipboard

Double click inside box below to view structure

wogonin - chemicalize.org - Windows Internet Explorer

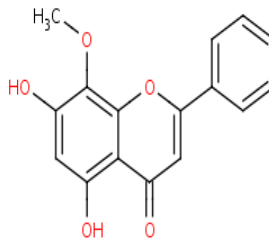
http://www.chemicalize.org/?mol=5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one

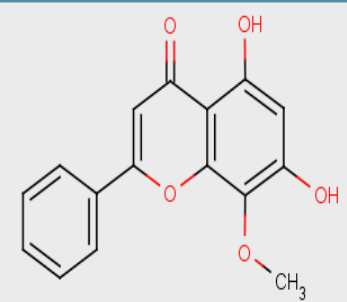
chemicalize.org<sup>beta</sup> Home ChemAxon Extend Feedback & Contact Changelog About

5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one

Instant JChem Create, explore and share chemical and non chemical data in local and remote databases, on your desktop.

Manage calculations Layout: Medicinal Chemist + Open All - Close All Download results

Molecule	Names and identifiers
	<p>Common names: wogonin</p> <p>IUPAC: 5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one</p> <p>Smiles: <chem>COC1=C2OC(=CC(=O)C2=C(O)C=C1O)C1=CC=CC=C1</chem></p> <p>InChI: <chem>InChI=1S/C16H12O5/c1-20-15-12(19)7-10(17)14-11(18)8-13(21-16(14)15)9-5-3-2-4-6-9/h2-8,17,19H,1H3</chem></p>
	<p>Elemental Analysis</p> <p>Formula: C<sub>16</sub>H<sub>12</sub>O<sub>5</sub></p> <p>Isotope formula: C<sub>16</sub>H<sub>12</sub>O<sub>5</sub></p> <p>Composition: C (67.5%), H (4.25%), O (28.25%)</p>



Copy to clipboard

Select/Deselect All

Transfer to Global Search

CWM GlobalSearch version 4.8.5.0

QuickSearch | QuickSearch Results | Global Search | Global Search Results

Clear Form | Clear Structure | Read Mol File | Read SDFFile | Read RXN File | Read RD File | Save Query | Load Query

Home | Feedback | Impressum

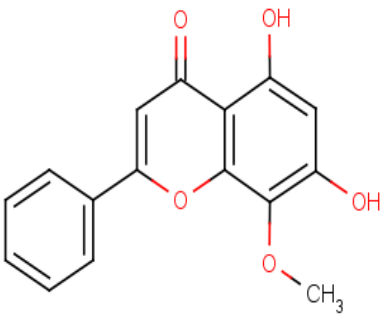
**CAS Registry number**

- 10-29-7
- 632-85-9

**Synonym name or free text**

- 5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one
- 5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one
- "4H-1-Benzopyran-4-one, 5,7-dihydroxy-8-methoxy-2-phenyl-"
- 5,7-Dihydroxy-8-methoxyflavone
- "5-18-04-00571 (Beilstein Handbook Reference)"
- AIDS001403
- AIDS-001403
- "BRN 0287152"
- C10197
- "FLAVONE, 5,7-DIHYDROXY-8-METHOXY-"
- NCI60\_040649
- "Norwogonin 8-methyl ether"
- NSC717845

Double click inside box below to open structure editor  
or right click inside box below and use edit>paste to paste structure



**Major datasources**

- Google
- PubChem
- ChemSpider
- Chemical Structure Lookup Service
- eMolecules
- NIST Webbook
- NCI Database

**Specialized datasources**

- Wikipedia
- SCIRUS
- ChemAxon Chemicalize Search
- ChemicalDB
- ChemicalBook
- ChemSynthesis
- ChemExper
- Buyersguide
- MOLPORT
- ZINC
- AKos Samples

**Options**

Structure Search

- Include isomers
- Include Substructures
- Include similar compounds

Similarity coefficient (1-100)

**Predefined profiles**

- Search in chemistry datasources
- Search in structure searchable datasources
- Find physical properties
- Find suppliers
- Find safety information
- Find spectra
- Find literature
- Find Open Access articles
- Find drug information

**My profiles**

# CWM Global Search

## The Global Search results page



CWM GlobalSearch version 4.8.5.0

QuickSearch QuickSearch Results Global Search Global Search Results

Save Result Load Result Home | Feedback | Impressum

GlobalSearchResultsPage.xaml?title=634403146025019526

Identifier	Number of links	Status	Message
RECORD_1	13	OK	Click leftmost button to expand/collapse results <span>chemicalize &gt;</span>

<input type="checkbox"/> Datasource	Result	Search type	Query	Errors
<input type="checkbox"/> ChemAxon Chemicalize Search	<a href="#">1 structure found</a>	FULLSTRUCTURE		
<input type="checkbox"/> GOOGLE	<a href="#">4 results</a>	FULLSTRUCTURE		
<input type="checkbox"/> GOOGLE	<a href="#">9 results</a>	FULLSTRUCTURE		
<input type="checkbox"/> GOOGLE	<a href="#">About 27 results</a>	FULLSTRUCTURE		
<input type="checkbox"/> GOOGLE	<a href="#">About 84 results</a>	FULLSTRUCTURE		
<input type="checkbox"/> GOOGLE	<a href="#">About 20,400 results</a>	CASNUMBER	632-85-9	
<input type="checkbox"/> GOOGLE	<a href="#">About 41,600,000 results</a>	CASNUMBER	10-29-7	
<input type="checkbox"/> GOOGLE	<a href="#">About 802 results</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one	
<input type="checkbox"/> GOOGLE	<a href="#">About 9,310 results</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one	
<input type="checkbox"/> WIKIPEDIA	<a href="#">Results 1-3 of 3</a>	FULLSTRUCTURE		
<input type="checkbox"/> WIKIPEDIA	<a href="#">Result 1 of 1</a>	CASNUMBER	632-85-9	
<input type="checkbox"/> WIKIPEDIA	<a href="#">Result 1 of 1</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one	
<input type="checkbox"/> WIKIPEDIA	<a href="#">Result 1 of 1</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one	

Open selected links in Browserwindow
  Show/Hide topics

# CWM Global Search

## The Global Search results drilldown



CWM GlobalSearch version 4.8.5.0

QuickSearch QuickSearch Results Global Search Global Search Results

Save Result Load Result

GlobalSearchResultsPage.xls

Identifier	Number of links	Status	Message
RECORD_1	13	OK	Click leftmost button to expand/collapse results <a href="#">chemicalize &gt;</a>

Datasource	Result	Search type	Query
ChemAxon Chemicalize Search	<a href="#">1 structure found</a>	FULLSTRUCTURE	
GOOGLE	<a href="#">4 results</a>	FULLSTRUCTURE	
GOOGLE	<a href="#">9 results</a>	FULLSTRUCTURE	
GOOGLE	<a href="#">About 27 results</a>	FULLSTRUCTURE	
GOOGLE	<a href="#">About 84 results</a>	FULLSTRUCTURE	
GOOGLE	<a href="#">About 20,400 results</a>	CASNUMBER	632-85-9
GOOGLE	<a href="#">About 41,600,000 results</a>	CASNUMBER	10-29-7
GOOGLE	<a href="#">About 802 results</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one
GOOGLE	<a href="#">About 9,310 results</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one
WIKIPEDIA	<a href="#">Results 1-3 of 3</a>	FULLSTRUCTURE	
WIKIPEDIA	<a href="#">Result 1 of 1</a>	CASNUMBER	632-85-9
WIKIPEDIA	<a href="#">Result 1 of 1</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenylchromen-4-one
WIKIPEDIA	<a href="#">Result 1 of 1</a>	SYNONYMNAME	5,7-dihydroxy-8-methoxy-2-phenyl-4H-chromen-4-one

Open selected links in Browserwindow Show/Hide topics

Search - chemicalize.org - Windows Internet Explorer

http://www.chemicalize.org/search

File Edit View Favorites Tools Help

Google

Search - chemicalize.org

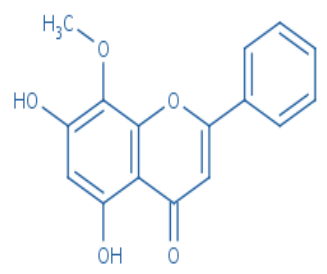
chemicalize.org beta

COc1c(cc(c2c1cc(cc2=O)c3ccccc3)O)O

draw upload Exact match ?

JChem for Excel Chemistry in Excel - Structure handling and visualizing capabilities within a Mic

1 structure found:



wogonin

Calculate Search

Pages: 28

SSS EXA SIM

created by ChemAxon

The chemicalize.org website including all name to structure and structure based calculations and predictions by ChemAxon is licensed under a Creative Commons License. Permissions beyond the scope of this license may be available at

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Internet | Protected Mode: On

100%

# CWM Global Search

## Using ChemAxon products and services in Silverlight



Where do I find CWM Global Search on the Internet ?

<http://cwmglobalsearch.com/gsweb>

Either request a 30 days trial key or use the free version

## How to find us on the internet or contact us ?

Our homepage

<http://www.akosgmbh.de>

CWM Global Search home page

<http://www.akosgmbh.de/globalsearch/index.htm>

Via eMail

[globalsearch@akosgmbh.de](mailto:globalsearch@akosgmbh.de)

***AKos***  
***Consulting & Solutions GmbH***



Thank you for your attention !

If you are interested in a live demonstration of CWM Global Search or if you are interested in implementation details of integrating ChemAxon Marvin and Services In Microsoft Silverlight applications ...

Please visit me at the exhibition area !