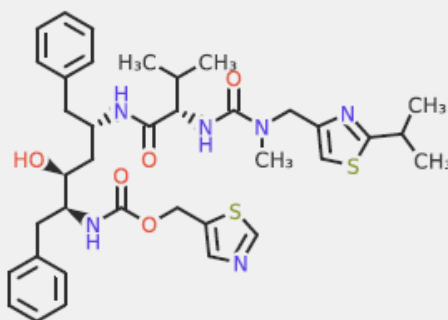


# Case 3:

Ritonavir



New Group 1 Specified Substance

New Substance

**Physical Forms**

**References**

**Physical Properties**

# Premise:

Fresh System

Ritonavir is not registered in any form

Referenced solvent substances are already registered

# Premise:

User wishes to register Ritonavir, which is a small molecule.

However, there are 2 relevant physical forms (different polymorphs) that the user would also like to register as Group 1 Specified Substances.

[Home](#)

[Search](#)

[Download](#)

[Register](#)

[Admin](#)



*Register New:*

Substance

Product



[Home](#)

[Search](#)

[Download](#)

[Register](#)

[Admin](#)



*Register New:*

Substance

Product

Single Substance

Mixture Substance

Specified Substance

Not Sure



[Home](#)

[Search](#)

[Download](#)

[Register](#)

[Admin](#)



*Register New:*

Substance

Product

Single Substance

Mixture Substance

Specified Substance

Not Sure

Chemical

Protein

Nucleic Acid

Structurally Diverse

Polymer



## Add Name

Name:

Ritonavir



Language:

English



Domain:

Drug



Name Type:

Common Name



Official Name

Systematic Name

Code

Common Name

Brand Name

Public Domain:



References

(0 references)

Cancel

Done

Please select a reference

## Add Name

Name:

Ritonavir



Language:

English



Domain:

Drug



Name Type:

Official Name



Public Domain:



Naming Org:

Deprecated:

INN



Official Jurisdiction:

US

NL

CA

DE



Add / Select References

(0 references)



Please select a reference.

Cancel

Done



# Select Reference(s)

*Type*

*Citation*

*URL*

*Uploaded*

*Date*

Add Reference



None selected

Cancel

Select

## Add Reference

*Type:*

INN List ▼

*Citation:*

Proposed List 74

*URL:*

[http://whqlibdoc.who.int/inn/proposed\\_lists/prop\\_INN\\_list74.pdf](http://whqlibdoc.who.int/inn/proposed_lists/prop_INN_list74.pdf)

*Upload:*



*Reference Date:*

04/26/2012



Cancel

Done

Select Reference(s)

	Type	Citation	URL	Uploaded	Date	
<input checked="" type="checkbox"/>	INN List	Proposed List 74	<a href="http://whqlibdoc.who...">http://whqlibdoc.who...</a>		04/2/2012	

Add Reference



1 selected

Cancel

Select

## Add Name

Name:

Ritonavir



Language:

English



Domain:

Drug



Name Type:

Official Name



Public Domain:



Naming Org:

Deprecated:

INN



Official Jurisdiction:

US

NL

CA

DE



Add / Select References

(1 reference)

Type

Citation

URL

INN List

Proposed List 74

<http://whqlibdoc.who...>



Cancel

Done

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)*Enter Names for Substance:*

Name:	Type:	Language:	Domain:	Preferred:
Ritonavir 	Official	English	Drug	<input checked="" type="checkbox"/> 
Ritonavirum	Official	Latin	Drug	<input type="checkbox"/> 
ритонавир	Official	Russian	Drug	<input type="checkbox"/> 
利托那韦	Official	Chinese	Drug	<input type="checkbox"/> 

 Structure available from name.

[Fetch Structures](#)

[Home](#) [Search](#) [Download](#) [Register](#) [Admin](#)

### Suggestions by Name:

By Source:

Any

[NCI Resolver](#)

1

[ChemIDPlus](#)

1

[PubChem](#)

1

[ChemSpider](#)

1

By Name:

Any

["Ritonavir"](#)

4

By Structure:

Any

[Structure 1](#)

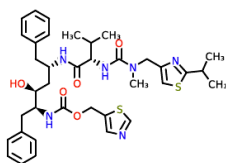
3

[Structure 2](#)

1

From **any** source, called **"Ritonavir"**, with **any** structure:

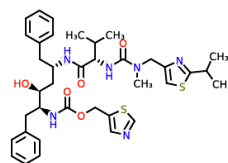
NCI Resolver



Ritonavir

[Choose](#)

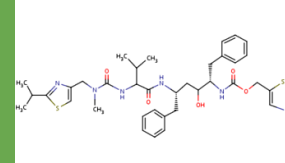
PubChem



Ritonavir

[Choose](#)

ChemIDPlus

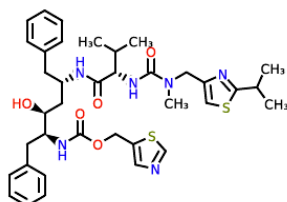


Ritonavir

[Choose](#)

4 Results

[Skip](#)

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)UNREGISTERED MOIETYMoiety **1** of **1**Defined Stereocenters: **4**Total Stereocenters: **4**E / Z centers: **0**Charge: **0**

Molecular Formula:

 $C_{37}H_{48}N_6O_5S_2$ 

Molecular Weight:

**720.946**

## Stereochemistry

## Optical Activity

Is there atropisomerism?

## Structure References

(1 reference)

Type

Citation





URL

PubChem

CID 392622

<http://pubchem.ncbi...>

## Select Reference(s)

	Type	Citation	URL	Uploaded	Date	
<input checked="" type="checkbox"/>	INN List	Proposed List 74	<a href="http://whqlibdoc.who...">http://whqlibdoc.who...</a>		04/26/2012	
<input checked="" type="checkbox"/>	Pubchem Record	CID 392622	<a href="http://pubchem.ncbi...">http://pubchem.ncbi...</a>		04/26/2012	
						<b>Add Reference</b> 

2 selected

Cancel

Select



## Add Reference

**Type:**

FAB Mass Spectrum

**Citation:**

Figure 2 in submitted document

**URL:**

**Upload:**

Ritonavir-Documentation-01-US.pdf



**Reference Date:**






04/26/2012



Cancel

Done

## Select Reference(s)

	Type	Citation	URL	Uploaded	Date	
<input checked="" type="checkbox"/>	INN List	Proposed List 74	<a href="http://whqlibdoc.who...">http://whqlibdoc.who...</a>		04/26/2012	
<input checked="" type="checkbox"/>	Pubchem Record	CID 392622	<a href="http://pubchem.ncbi...">http://pubchem.ncbi...</a>		04/26/2012	
<input checked="" type="checkbox"/>	FAB Mass Spectrum	Figure 2 in submitted document.			04/26/2012	

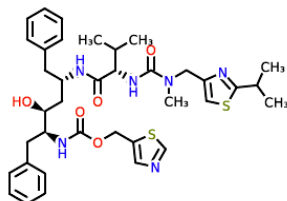
Add Reference



2 selected

Cancel

Select

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)UNREGISTERED MOIETYMoiety **1** of **1**Defined Stereocenters: **4**Total Stereocenters: **4**E / Z centers: **0**Charge: **0**

Molecular Formula:

 $C_{37}H_{48}N_6O_5S_2$ 

Molecular Weight:

**720.946**

## Stereochemistry

Achiral

**Absolute**

Mixed

Racemic

Epimeric

Unknown

## Optical Activity

( + / - )

( + )

( - )

None

**Unspecified**Is there atropisomerism?

Yes

**No**

## Structure References (3)

**Type****Citation****URL**

PubChem

CID 392622

<http://pubchem.ncbi...>

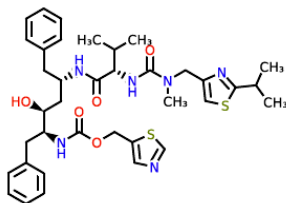
INN List

Proposed List 74

<http://whqlibdoc.who...>

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

### Ready to Register new Substance

**Absolute****Molecular Formula:****C<sub>37</sub>H<sub>48</sub>N<sub>6</sub>O<sub>5</sub>S<sub>2</sub>****Molecular Weight:****720.946****Defined Stereocenters:** **4****Total Stereocenters:** **4****E / Z centers:** **0****Charge:** **0****Names** **9****References** **6****Relationships** **0****Notes** **0****Properties** **0****Name****Lang.****Dom.****Type****Preferred:**

Ritonavir

English

Drug

Official



Ritonavirum

Latin

Drug

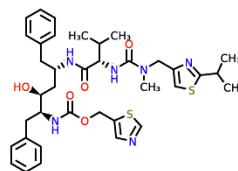
Official

[Register Substance](#)

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

Successfully submitted *Single Chemical Substance*:

SUBST\_F1UPQ



**Absolute**

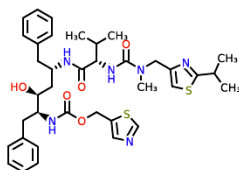
Ritonavir

Is there a more specific physical form of this substance?



[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

Constituents:

SUBST F1UPQ**Absolute**

Ritonavir

Component ▼

Add New  
Constituent

Choose

Names

Amounts

Properties

References

Notes

Add Name



Register

## Add Name

*Name:*

Ritonavir Form I

*Language:*

English



*Domain:*

Drug



*Name Type:*

Common Name



*Public Domain:*



Add / Select References

(0 references)



Please select a reference.

Cancel

Done

# Select Reference(s)

*Type*

*Citation*

*URL*

*Uploaded*

*Date*

Add Reference



None selected

Cancel

Select



## Add Reference

*Type:*

Journal Article ▼

*Citation:*

Pharmaceutical Research, Vol. 18, No. 6, 2001

*URL:*

<http://link.springer.com/content/pdf/10.1023%2FA%3A1011052932607.pdf>

*Upload:*



*Reference Date:*



04/26/2012



Cancel

Done

# Select Reference(s)

	Type	Citation	URL	Uploaded	Date	
<input checked="" type="checkbox"/>	Journal Article	Pharmaceutical Research	<a href="http://link.springer.com...">http://link.springer.com...</a>		04/26/2012	

Add Reference



1 selected

Cancel

Select

## Add Name

*Name:*

Ritonavir Form I

*Language:*

English



*Domain:*

Drug



*Name Type:*

Common Name



*Public Domain:*



Add / Select References

(1 reference)

*Type*

*Citation*

*URL*

Journal Article

Pharmaceutical Research

<http://link.springer.com...>



Cancel

Done

SUBST F1UPQ



## Choose

## Component

## Notes

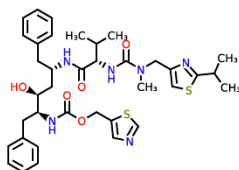
**Preferred:**

☒

## Register

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

Constituents:

SUBST\_F1UPQ**Absolute**

Ritonavir

Add New  
Constituent

Choose

Component ▼

Names (1)

Amounts

Properties

References (1)

Notes

Add Property



Register

## Add Property

**Property:**

<Property>

**Value:**

Melting Point

**Conditions:**

Solubility:Quantitative

Solubility:Qualitative

Physical Form : State

**Notes:**

...

**References:**

Add / Select References

Cancel

Done

## Add Property

**Property:**

Solubility: Quantitative ▼

**Value:**

**Solvent:**

Water ▼

**Avg: Low: High:**

**Solubility:**

g/mL

**Conditions:**

**Notes:**

**References:**

Add / Select References

Cancel

Done

## Add Property

**Property:**

Solubility: Quantitative ▼

**Value:**

**Solvent:**

Water ▼

Water

**Solubility:**

Ethanol

g/mL

Methanol

**Conditions:**

Choose Substance

**Notes:**

**References:**

Add / Select References

Cancel

Done



## Select Solvent

Substances matching "Water Ethanol" with tag "solvent"



SSUB\_1254F

H<sub>2</sub>O

HO-CH<sub>3</sub>

Ethanol/Water 99/1

SSUB\_65H4W

H<sub>2</sub>O

HO-CH<sub>3</sub>

Ethanol/Water 90/10

SSUB\_8UA92

H<sub>2</sub>O

HO-CH<sub>3</sub>

Ethanol/Water 75/25

10 Results

## Add Property

**Property:**

Solubility: Quantitative ▼

**Value:**

**Solvent:**

Ethanol/Water 99/1 ▼

SSUB\_1254F

**Avg: Low: High:**

**Solubility:**

188

g/mL

**Conditions:**

5 Degrees C

**Notes:**



**References:**

Add / Select References

Cancel

Done

# Select Reference(s)

	Type	Citation	URL	Uploaded	Date	
<input checked="" type="checkbox"/>	Journal Article	Pharmaceutical Research	<a href="http://link.springer.com...">http://link.springer.com...</a>		04/26/2012	

Add Reference



1 selected

Cancel

Select

## Add Property

**Property:**

Solubility: Quantitative

**Value:**

**Solvent:**

Ethanol/Water 99/1

SSUB\_1254F

**Solubility:**

**Avg:** **Low:** **High:**

188

g/mL

**Conditions:**

5 Degrees C

**Notes:**

**References (1):**

Add / Select References

**Type**

**Citation**

**URL**

Journal Article

Pharmaceutical Research

<http://link.springer.com...>

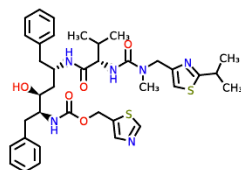


Cancel

Done

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

## Constituents:

SUBST\_F1UPQ

Absolute

Ritonavir

Add New  
Constituent

Choose

Component ▼

Names (1)

Amounts

Properties (1)

References (1)

Notes

Property:

Value:

Conditions:

Notes:

Defining: 

Solubility:Quantitative

188 g/mL in SSUB\_1254F

5 Degrees C



Add Property

Register 

## Add Property

***Property:***

Physical Form : State ▼

***Value:***

Solid ▼

***Conditions:***

***Notes:***

***References:***

Add / Select References

Cancel

Done

## Register

## Add Property

**Property:**

Physical Form : Crystallographic Space Group ▼

**Value:**

#4 : monoclinic : P2<sub>1</sub> ▼

**Conditions:**

**Notes:**

**References:**

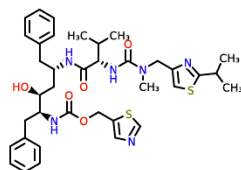
Add / Select References

Cancel

Done



## Register

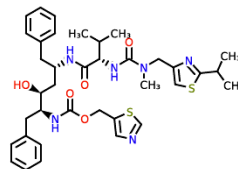


[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

Successfully submitted *Group 1 Specified Substance:*

SUBST\_97RUZ

Solid;  
Monoclinic P2<sub>1</sub>



Absolute

Ritonavir Form I

Is there another form of the parent substance?



Would you like to use SUBST\_97RUZ as a starting template?



SUBST F1UPQ



## Add New Constituent

## Choose

## Component

## Names (1)

## Properties (3)

## References (1)

## Notes

**Name:**

**Type:**

**Language:**

**Domain:**

**Preferred:**

# Ritonavir Form I

## Common

English

Drug



## Add Name

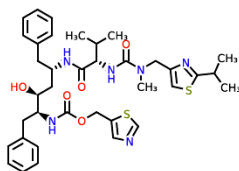


## Register



[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

## Constituents:

SUBST\_F1UPQ**Absolute**

Ritonavir

Component

Add New  
Constituent

Choose

Names

Amounts

Properties (3)

References (1)

Notes

Add Name



Register

## Register

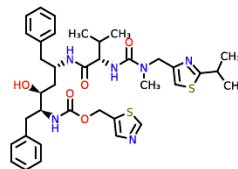
☒

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)

Successfully submitted *Group 1 Specified Substance:*

SUBST\_48UTE

Solid;  
orthorhombic : P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>



**Absolute**

Ritonavir Form II

Is there another form of the parent substance?

Yes

No

