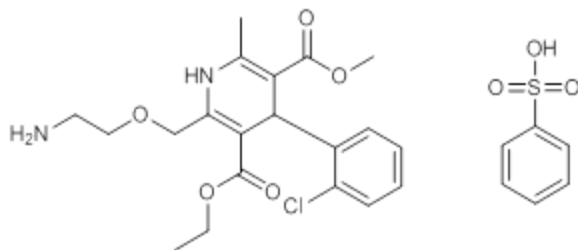


Case 1:

Amlodipine Besylate



Official Name

Salt / Parent Relationship

Approved Drug

Chemical Substance

Premise:

Empty System

No substances present

No references present

Entering Salt form before Parent Moiety, or other related substances.

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Register New:

Substance

Specified Substance

Product

Application



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Register New:

Substance

Specified Substance

Product

Application

Chemical

Protein

Nucleic Acid

Structurally Diverse

Mixture



[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)*Name:*

Amlodipine Besylate

*Language:*

English

*Domain:*

Drug

*Name Type:*

Common Name

*Public Domain:**Source:*

Official Name

Source:

SOURCE

Systematic Name

Code

Common Name

*Source Doc:**Source Date:*

04/11/2012



[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)*Name:*

Amlodipine Besylate

*Language:*

English

*Domain:*

Drug

*Name Type:*

Official Name

*Public Domain:**Naming Org:*

INN

*Deprecated:**Deprecated Date:*

N/A

*Official Jurisdiction:*

US

NL

*Source:**Source:*

Martindale

*Source-URL:*

http://example.com

Source Doc:

DOC_123.pdf

*Source Date:*

04/11/2012



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

Name:	Type:	Language:	Domain:	Preferred:
Amlodipine Besylate 	Official	English	Drug	<input checked="" type="checkbox"/> 
Амлодипина Безилат	Official	Russian	Drug	<input type="checkbox"/> 
3-O-ethyl 5-O-met... 	Systematic	English	Drug	<input type="checkbox"/> 
				

 Structure available from name.

[Fetch Structures](#)

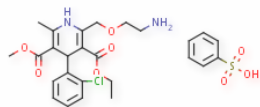
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Found from other sources:

"Amlodipine Besylate" (3)

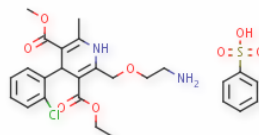
"3-O-ethyl 5-O-met..." (1)

NCI Resolver



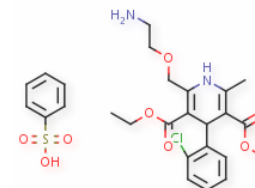
Choose

PubChem



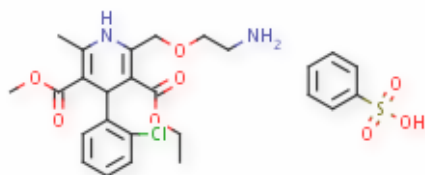
Choose

ChemSpider



Choose

Skip

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Defined Stereocenters: 0

Total Stereocenters: 1

E / Z centers: 0

Charge: 0

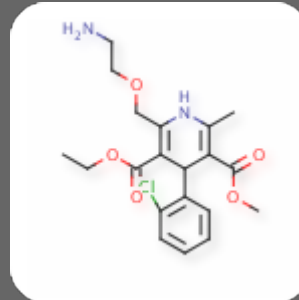
Molecular Formula:

 $\text{C}_{20}\text{H}_{25}\text{ClN}_2\text{O}_5 \cdot \text{C}_6\text{H}_6\text{O}_3\text{S}$

Molecular Weight:

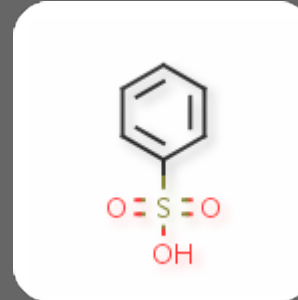
408.879 • 158.18

There are 2 moieties for this compound:

UNREGISTERED

Moiety 1

x 1

UNREGISTERED

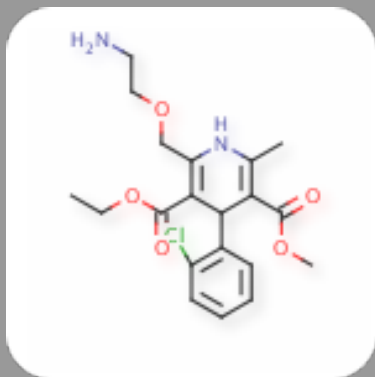
Moiety 2

x 1

Is the stoichiometry fixed as shown?

Fixed

Variable

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)UNREGISTERED MOIETYMoiety **1** of **2**

Defined Stereocenters: 0

Total Stereocenters: 1

E / Z centers: 0

Charge: 0

Molecular Formula:

 $C_{20}H_{25}ClN_2O_5$

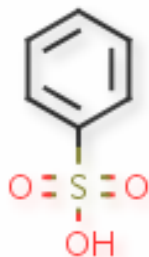
Molecular Weight:

408.879

Stereochemistry

Optical Activity

Is there additional stereochemistry?

[Home](#)[Search](#)[Download](#)[Register](#)[Admin](#)UNREGISTERED MOIETYMoiety **2** of **2**

Defined Stereocenters: 0

Total Stereocenters: 0

E / Z centers: 0

Charge: 0

Molecular Formula:

 $\text{C}_6\text{H}_6\text{O}_3\text{S}$

Molecular Weight:

158.18

Stereochemistry

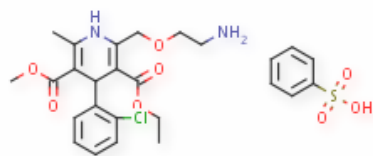
[Achiral](#)[Absolute](#)[Mixed](#)[Racemic](#)[Epimeric](#)[Unknown](#)

Optical Activity

[\(+/-\)](#)[\(+\)](#)[\(-\)](#)[None](#)[Unknown](#)Is there additional stereochemistry?[Yes](#)[No](#)

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Ready to Register new Substance

**Racemic****Molecular Formula:** $C_{20}H_{25}ClN_2O_5 \cdot C_6H_6O_3S$ **Molecular Weight:**

408.879 • 158.18

Defined Stereocenters:0 (**Racemic**)**Total Stereocenters:**

1

E / Z centers:

0

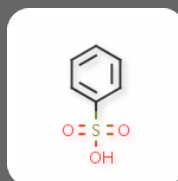
Charge:

0

Moieties (2)

Unregistered**Racemic****Moiety 1**

x1

Unregistered**Moiety 2**

x1

Names (3)

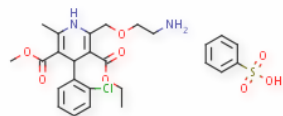
Name	Lang.	Dom.	Type	Pref
Amlodipine Besylate	English	Drug	Official	<input checked="" type="checkbox"/> 
Амлодипина Безилат	Russian	Drug	Official	<input type="checkbox"/> 

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Successfully Registered:

SUBST_DXQQ42

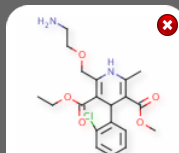


Racemic

Amlodipine Besylate

Suggested New Derived Substances:

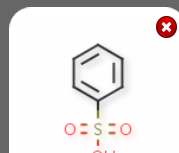
Moiety 1



Racemic

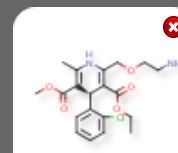
Racemic

Moiety 2



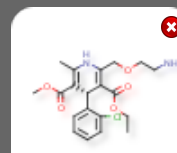
Achiral

Moiety 1 (R)-
Isomer



Absolute

Moiety 1
(S)-Isomer



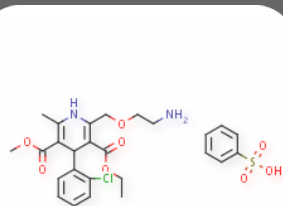
Absolute

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Successfully Registered:

SUBST_DXQQ42

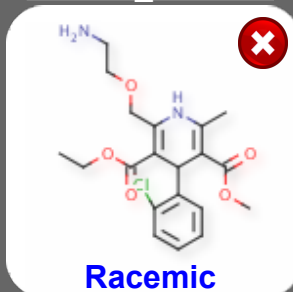


Racemic

Amlodipine Besylate

New Relationships:

SUBST_RTQ421



Racemic

Amlodipine

is a

Parent

of SUBST_DXQQ42

SUBST_Y59GR4



Benzosulphonic Acid

is a

Parent

of SUBST_DXQQ42

New

Choose

Save Relationships