

## COMPOUND SUMMARY

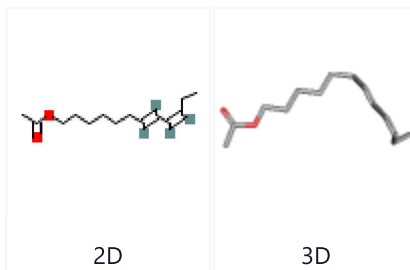
# 7,9-Dodecadienyl acetate, (7E,9Z)-

[Cite](#)[Download](#)

PubChem CID

1794807

Structure



Chemical Safety



Irritant

Environmental  
Hazard[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula

C<sub>14</sub>H<sub>24</sub>O<sub>2</sub>

Synonyms

7,9-Dodecadienyl acetate, (7E,9Z)-  
[(7E,9Z)-dodeca-7,9-dienyl] acetate  
7E,9Z-Dodecadienyl acetate  
trans-7,cis-9-Dodecadienyl acetate  
ODG58N4V3J

[View More...](#)**Molecular Weight**

224.34 g/mol

*Computed by PubChem 2.2 (PubChem release 2025.04.14)***Dates**

Create: 2005-03-27    Modify: 2025-05-18

**Description**

7E,9Z-Dodecadienyl acetate is a carboxylic ester.

[▶ ChEBI](#)

[7,9-Dodecadienyl acetate, \(7E,9Z\)-](#) has been reported in [Lobesia botrana](#) with data available.

[▶ LOTUS - the natural products occurrence database](#)

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11 Biological Test Results



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## 1 Structures



### 1.1 2D Structure



Chemical Structure Depiction

Search, image, and download icons

Fullscreen and zoom in icons



► PubChem

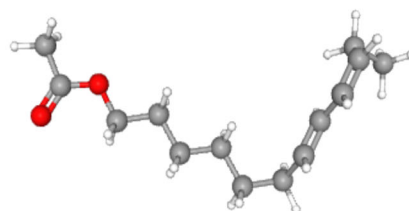
## 1.2 3D Conformer



### Interactive Chemical Structure Model

Ball and Stick  Sticks  Wire-Frame  Space-Filling

Show Hydrogens  Animate



« First < Previous Conformer 1 of 10 Next > Last »»

[▶ PubChem](#)

## 2 Names and Identifiers



### 2.1 Computed Descriptors



#### 2.1.1 IUPAC Name



[(7E,9Z)-dodeca-7,9-dienyl] acetate

*Computed by Lexichem TK 2.7.0 (PubChem release 2025.04.14)*

[▶ PubChem](#)

#### 2.1.2 InChI



InChI=1S/C14H24O2/c1-3-4-5-6-7-8-9-10-11-12-13-16-14(2)15/h4-7H,3,8-13H2,1-2H3/b5-4-,7-6+

*Computed by InChI 1.07.2 (PubChem release 2025.04.14)*

[▶ PubChem](#)

#### 2.1.3 InChIKey



LLRZUAWETKPZJO-SCFJQAPRSA-N

*Computed by InChI 1.07.2 (PubChem release 2025.04.14)*

[▶ PubChem](#)

## 2.1.4 SMILES



CC/C=C\C=C\CCCCCOC(=O)C

Computed by OEChem 2.3.0 (PubChem release 2025.04.14)

▶ [PubChem](#)

## 2.2 Molecular Formula



C<sub>14</sub>H<sub>24</sub>O<sub>2</sub>

Computed by PubChem 2.2 (PubChem release 2025.04.14)

▶ [PubChem](#)

## 2.3 Other Identifiers



### 2.3.1 CAS



54364-62-4

▶ [CAS Common Chemistry](#); [ChemIDplus](#); [EPA Chemicals under the TSCA](#); [EPA DSSTox](#); [European Chemicals Agency \(ECHA\)](#); [FDA Global Su...](#)

### 2.3.2 European Community (EC) Number



259-127-7

▶ [European Chemicals Agency \(ECHA\)](#)

### 2.3.3 UNII



ODG58N4V3J

- ▶ FDA Global Substance Registration System (GSRS)

### 2.3.4 ChEBI ID



CHEBI:196041

- ▶ ChEBI

### 2.3.5 DSSTox Substance ID



DTXSID301014954

- ▶ EPA DSSTox

### 2.3.6 Lipid Maps ID (LM\_ID)



LMFA07010239

- ▶ LIPID MAPS

### 2.3.7 Metabolomics Workbench ID



3884

▶ Metabolomics Workbench

## 2.3.8 Wikidata



Q27285589

▶ Wikidata

## 2.4 Synonyms



### 2.4.1 Depositor-Supplied Synonyms



7,9-Dodecadienyl acetate, (7E,9Z)-	AI3-36734	(7E,9Z)-7,9-Dodecadien-1-ol, 1-Acetate (~80%)	trans-7, cis
[(7E,9Z)-dodeca-7,9-dienyl] acetate	DODECADIENYL ACETATE, (E)7-(Z)9-	SCHEMBL702674	CS-0199159
7E,9Z-Dodecadienyl acetate	7,9-Dodecadien-1-ol, acetate, (7E,9Z)-	(E)7-(Z)9-dodecadienyl acetate	E76567
trans-7,cis-9-Dodecadienyl acetate	((7E,9Z)-dodeca-7,9-dienyl) acetate	CHEBI:196041	7E, 9Z-Doc
ODG58N4V3J	54364-62-4	LLRZUAWETKPZJO-SCFJQAPRSA-N	Q27285589
EUDEMONE	(7E,9Z)-dodeca-7,9-dien-1-yl acetate	DTXSID301014954	TRANS-7, C
CCRIS 9116	(7Z,9E)-Dodeca-7,9-dienyl acetate	LMFA07010239	
EINECS 259-127-7	(7e,9z)-7,9-dodecadien-1-yl acetate	AKOS022186339	
7,9-Dodecadien-1-ol, 1-acetate, (7E,9Z)-	UNII-ODG58N4V3J	FD46802	
7,9-Dodecadien-1-ol, acetate, (Z,E)-	(7E,9Z)-7,9-Dodecadienyl acetate	BS-50825	

▶ PubChem

## 3 Chemical and Physical Properties



## 3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	224.34 g/mol	Computed by PubChem 2.2 (PubChem release 2025.04.14)
XLogP3-AA	4.3	Computed by XLogP3 3.0 (PubChem release 2025.04.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Rotatable Bond Count	10	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Exact Mass	224.177630004 Da	Computed by PubChem 2.2 (PubChem release 2025.04.14)
Monoisotopic Mass	224.177630004 Da	Computed by PubChem 2.2 (PubChem release 2025.04.14)
Topological Polar Surface Area	26.3 Å <sup>2</sup>	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Heavy Atom Count	16	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	217	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Isotope Atom Count	0	Computed by PubChem

Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	2	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2025.04.14)

► [PubChem](#)

## 3.2 Chemical Classes



### 3.2.1 Lipids



Fatty Acyls [FA] -> Fatty esters [FA07] -> Short fatty esters [FA0710]

► [LIPID MAPS](#)

## 4 Spectral Information



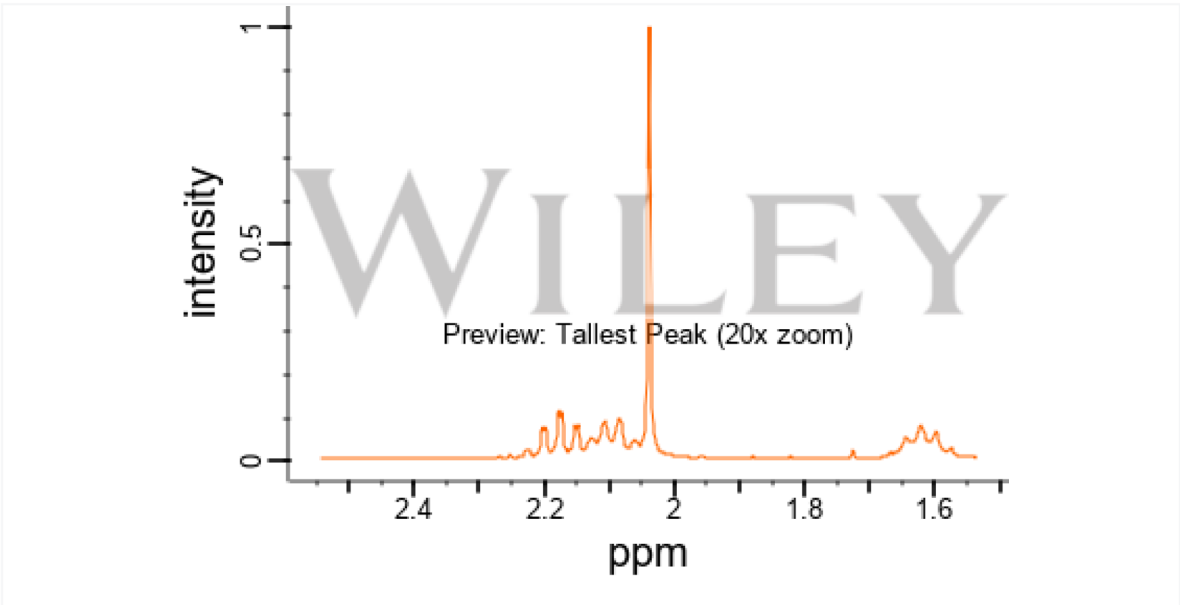
### 4.1 1D NMR Spectra



#### 4.1.1 1H NMR Spectra



Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.

Catalog Number	249203
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Thumbnail	

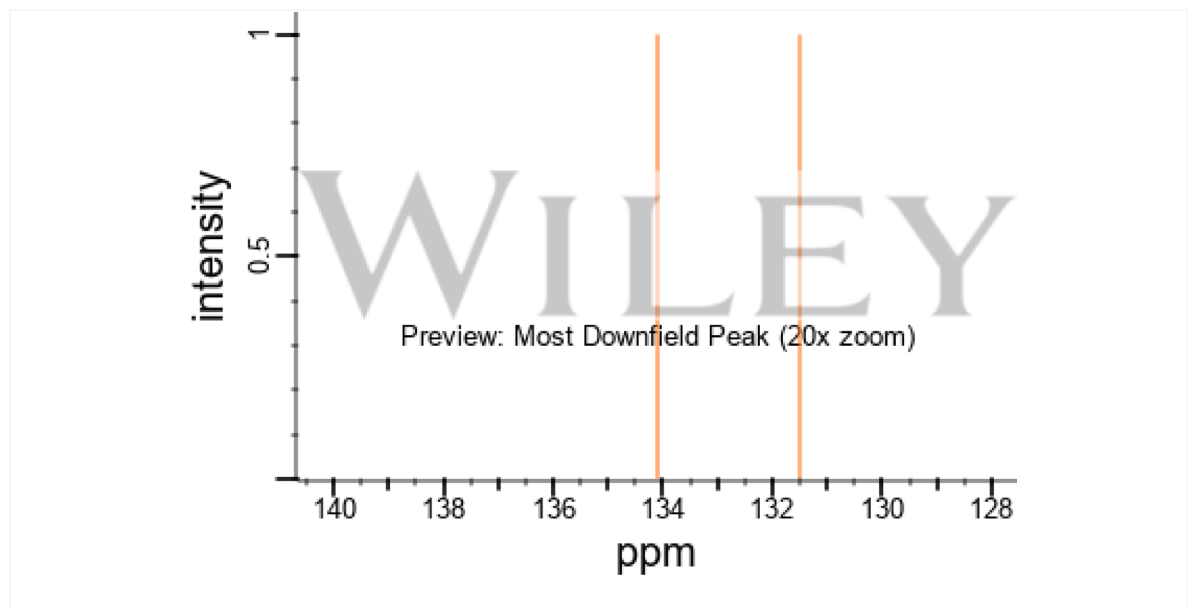
► [SpectraBase](#)

## 4.1.2 <sup>13</sup>C NMR Spectra



Instrument Name	VARIAN XL-100
Copyright	Copyright © 2002-2025 Wiley-VCH GmbH. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

## 4.2 Mass Spectrometry



### 4.2.1 GC-MS



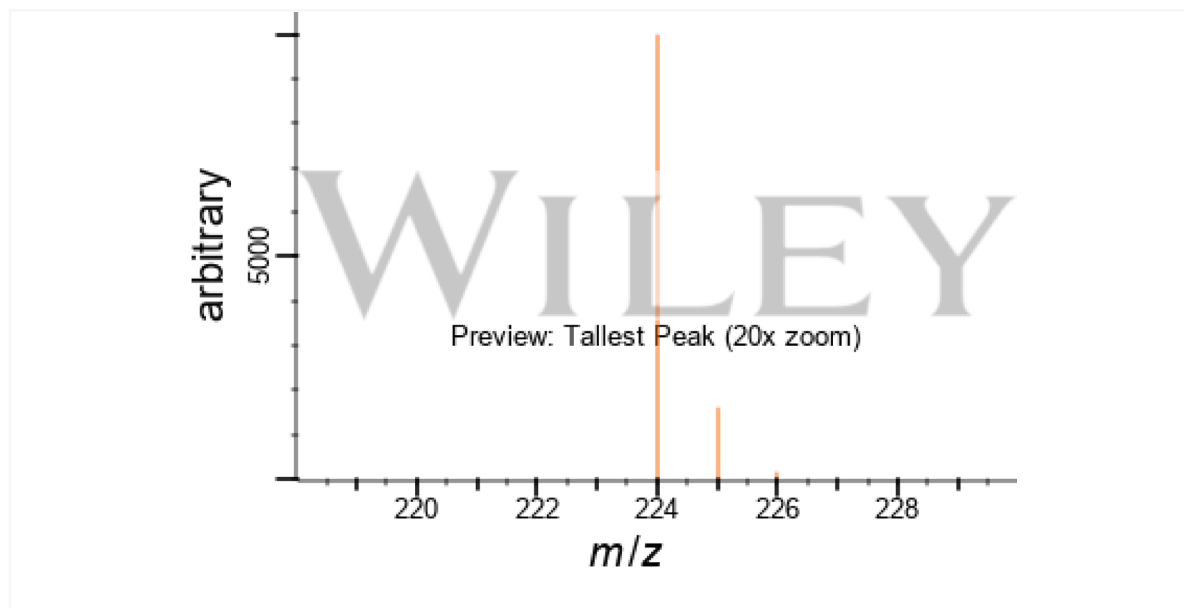
Source of Spectrum

F-43-870-3

Copyright

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## Thumbnail



► [SpectraBase](#)

## 4.3 IR Spectra

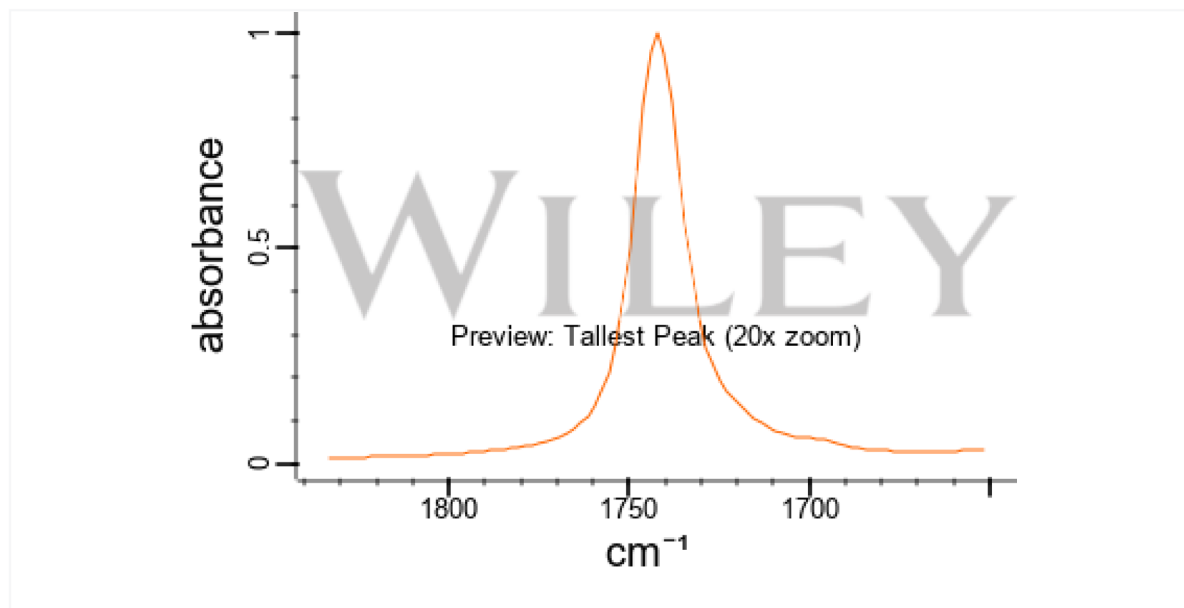


### 4.3.1 FTIR Spectra



Instrument Name	Bruker IFS 85
Technique	Film
Copyright	Copyright © 1989, 1990-2025 Wiley-VCH GmbH. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

## 4.4 Raman Spectra



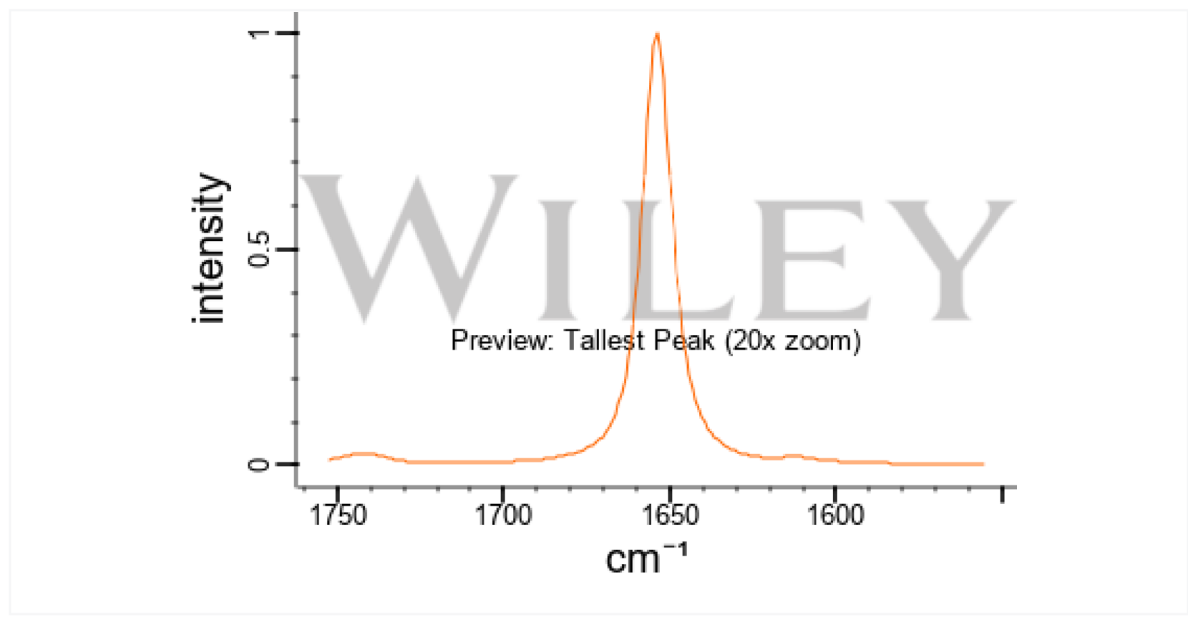
Catalog Number

249203

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Thumbnail

[▶ SpectraBase](#)

## 5 Related Records



### 5.1 Related Compounds with Annotation



Follow these links to [do a live 2D search](#) or [do a live 3D search](#) for this compound, sorted by annotation score. This section is deprecated (see [here](#) for details), but these live search links provide equivalent functionality to the table that was previously shown here.

[▶ PubChem](#)

### 5.2 Related Compounds



Same Connectivity Count

9

Same Parent, Connectivity Count	9
Mixtures, Components, and Neutralized Forms Count	1
Similar Compounds (2D)	<a href="#">View in PubChem Search</a>
Similar Conformers (3D)	<a href="#">View in PubChem Search</a>

▶ [PubChem](#)

## 5.3 Substances



### 5.3.1 PubChem Reference Collection SID



505540634

▶ [PubChem](#)

### 5.3.2 Related Substances



All Count	65
Same Count	64
Mixture Count	1

▶ [PubChem](#)

### 5.3.3 Substances by Category





▶ PubChem

## 6 Chemical Vendors

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▶ [PubChem](#)

## 7 Use and Manufacturing



### 7.1 General Manufacturing Information



#### EPA TSCA Commercial Activity Status

[7,9-Dodecadien-1-ol, 1-acetate, \(7E,9Z\)-](#): ACTIVE

▶ [EPA Chemicals under the TSCA](#)

## 8 Safety and Hazards





### 8.1 Hazards Identification



#### 8.1.1 GHS Classification



Pictogram(s)	  Irritant      Environmental Hazard
Signal	<b><u>Warning</u></b>
GHS Hazard Statements	H315 (91.7%): Causes skin irritation [ <b><u>Warning</u></b> Skin corrosion/irritation] H319 (15.1%): Causes serious eye irritation [ <b><u>Warning</u></b> Serious eye damage/eye irritation]

	<p>H400 (19.3%): Very toxic to aquatic life [<b>Warning</b> Hazardous to the aquatic environment, acute hazard]</p> <p>H410 (19.3%): Very toxic to aquatic life with long lasting effects [<b>Warning</b> Hazardous to the aquatic environment, long-term hazard]</p> <p>H411 (77.1%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]</p>
<b>Precautionary Statement Codes</b>	<p>P264, P264+P265, P273, P280, P302+P352, P305+P351+P338, P321, P332+P317, P337+P317, P362+P364, P391, and P501</p> <p>(The corresponding statement to each P-code can be found at the <a href="#">GHS Classification</a> page.)</p>
<b>ECHA C&amp;L Notifications Summary</b>	<p><i>Aggregated GHS information provided per 192 reports by companies from 6 notifications to the ECHA C&amp;L Inventory. Each notification may be associated with multiple companies.</i></p> <p><i>Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown. For more detailed information, please visit <a href="#">ECHA C&amp;L website</a>.</i></p>

► [European Chemicals Agency \(ECHA\)](#)

## 8.1.2 Hazard Classes and Categories



Skin Irrit. 2 (91.7%)

Eye Irrit. 2 (15.1%)

Aquatic Acute 1 (19.3%)

Aquatic Chronic 1 (19.3%)

Aquatic Chronic 2 (77.1%)

► [European Chemicals Agency \(ECHA\)](#)

## 9 Literature



## 9.1 Consolidated References

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▶ [PubChem](#)

## 9.2 Springer Nature References

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▶ Springer Nature

## 9.3 Thieme References

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▶ Thieme Chemistry

## 9.4 Chemical Co-Occurrences in Literature

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▶ PubChem

## 9.5 Chemical-Gene Co-Occurrences in Literature

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▶ PubChem

## 9.6 Chemical-Organism Co-Occurrences in Literature

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▶ PubChem

## 10 Patents

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### 10.1 Depositor-Supplied Patent Identifiers

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▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

## 10.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=LLRZUAWETKPZJO-SCFJQAPRSA-N>

▶ PATENTSCOPE (WIPO)

Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=LLRZUAWETKPZJO-GSLHJPOASA-N>

▶ PATENTSCOPE (WIPO)

## 10.3 Chemical Co-Occurrences in Patents





▶ [PubChem](#)

## 10.4 Chemical-Disease Co-Occurrences in Patents

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▶ PubChem

## 10.5 Chemical-Organism Co-Occurrences in Patents

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▶ PubChem

## 11 Biological Test Results

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### 11.1 BioAssay Results

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▶ PubChem

## 12 Taxonomy

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▶ LOTUS - the natural products occurrence database

## 13 Classification

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### 13.1 ChEBI Ontology

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▶ ChEBI

### 13.2 LIPID MAPS Classification

---



▶ LIPID MAPS

### 13.3 ChemIDplus

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▶ ChemIDplus

### 13.4 UN GHS Classification

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▶ GHS Classification (UNECE)

## 13.5 EPA DSSTox Classification



▶ EPA DSSTox

## 13.6 EPA TSCA and CDR Classification

---



▶ EPA Chemicals under the TSCA

## 13.7 LOTUS Tree

---



▶ [LOTUS - the natural products occurrence database](#)

## 13.8 EPA Substance Registry Services Tree



▶ [EPA Substance Registry Services](#)

## 13.9 MolGenie Organic Chemistry Ontology





▶ MolGenie

## 13.10 Chemicals in PubChem from Regulatory Sources

---



► PubChem

## 14 Information Sources



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### 1. CAS Common Chemistry

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*7E,9Z-Dodecadienyl acetate*

[https://commonchemistry.cas.org/detail?cas\\_rn=54364-62-4](https://commonchemistry.cas.org/detail?cas_rn=54364-62-4)

### 2. ChemIDplus

#### LICENSE

<https://www.nlm.nih.gov/copyright.html>

*7,9-Dodecadienyl acetate, (7E,9Z)-*

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0054364624>

*ChemIDplus Chemical Information Classification*

<https://pubchem.ncbi.nlm.nih.gov/source/chemidplus>

### 3. EPA Chemicals under the TSCA

#### LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

*7,9-Dodecadien-1-ol, 1-acetate, (7E,9Z)-*

<https://www.epa.gov/chemicals-under-tsca>

*EPA TSCA Classification*

<https://www.epa.gov/tscainventory>

#### 4. EPA DSSTox

##### LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

*(7Z,9E)-Dodeca-7,9-dienyl acetate*

<https://comptox.epa.gov/dashboard/DTXSID301014954>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

#### 5. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

*(7E,9Z)-dodecadienyl acetate*

<https://echa.europa.eu/substance-information/-/substanceinfo/100.053.734>

*(7E,9Z)-dodecadienyl acetate (EC: 259-127-7)*

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/71900>

#### 6. FDA Global Substance Registration System (GSRS)

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<https://www.fda.gov/about-fda/about-website/website-policies#linking>

*7,9-DODECADIENYL ACETATE, (7E,9Z)-*

<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/ODG58N4V3J>

#### 7. ChEBI

*7E,9Z-Dodecadienyl acetate*

<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:196041>

*ChEBI Ontology*

<http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology>

## 8. **LOTUS - the natural products occurrence database**

### LICENSE

The code for LOTUS is released under the GNU General Public License v3.0.

<https://lotus.nprod.net/>

*7,9-Dodecadienyl acetate, (7E,9Z)-*

<https://www.wikidata.org/wiki/Q27285589>

*LOTUS Tree*

<https://lotus.naturalproducts.net/>

## 9. **LIPID MAPS**

*SFE 14:2*

<https://lipidmaps.org/databases/lmsd/LMFA07010239>

*Lipid Classification*

<https://www.lipidmaps.org/>

## 10. **Metabolomics Workbench**

*7E,9Z-Dodecadienyl acetate*

<https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=3884>

## 11. **SpectraBase**

*Dodecadien-1-yl acetate, (7E,9Z)-*

<https://spectrabase.com/spectrum/CEXU5IT3rfa>

*7,9-DODECADIEN-1-OL ACETATE*

<https://spectrabase.com/spectrum/8jNaNTT31m5>

*trans-7, cis-9-Dodecadienyl acetate*

<https://spectrabase.com/spectrum/GX7YLvh5KYK>

*trans-7, cis-9-Dodecadienyl acetate*

<https://spectrabase.com/spectrum/GPeJR4EYMNS>

7,9-Dodecadien-1-ol, acetate, (Z,E)-

<https://spectrabase.com/spectrum/H4koeuJ3n28>

## 12. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/341249598>

## 13. Thieme Chemistry

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<https://pubchem.ncbi.nlm.nih.gov/substance/376781289>

## 14. Wikidata

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(7E,9Z)-7,9-dodecadienyl acetate

<https://www.wikidata.org/wiki/Q27285589>

## 15. PubChem

<https://pubchem.ncbi.nlm.nih.gov>

*Chemicals in PubChem from Regulatory Sources*

## 16. GHS Classification (UNECE)

*GHS Classification*

[http://www.unece.org/trans/danger/publi/ghs/ghs\\_welcome\\_e.html](http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)

## 17. EPA Substance Registry Services

### LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

*EPA SRS List Classification*

<https://maldi.nist.gov>

## 18. MolGenie

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*MolGenie Organic Chemistry Ontology*

<https://github.com/MolGenie/ontology/>

## 19. PATENTSCOPE (WIPO)

*SID 388439909*

<https://pubchem.ncbi.nlm.nih.gov/substance/388439909>

*SID 461720059*

<https://pubchem.ncbi.nlm.nih.gov/substance/461720059>