 Compound Summary for CID 596375[PUBCHEM](#) > [COMPOUND](#) > [CHAVIBETOL](#)

Chavibetol

[▶ Cite this Record](#)

Vendors



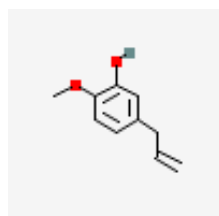
Literature



Patents



Bioactivities



PubChem CID:	596375
Chemical Names:	Chavibetol; M-Eugenol; 501-19-9; Phenol, 5-allyl-2-methoxy-; 2-methoxy-5-prop-2-enyl-phenol; 2-methoxy-5-(prop-2-en-1-yl)phenol More...
Molecular Formula:	$C_{10}H_{12}O_2$
Molecular Weight:	164.20108 g/mol
InChI Key:	NPBVQXIMTZKSBA-UHFFFAOYSA-N
UNII:	OE7NQ16G4D
Modify Date:	2015-08-08
Create Date:	2005-03-27

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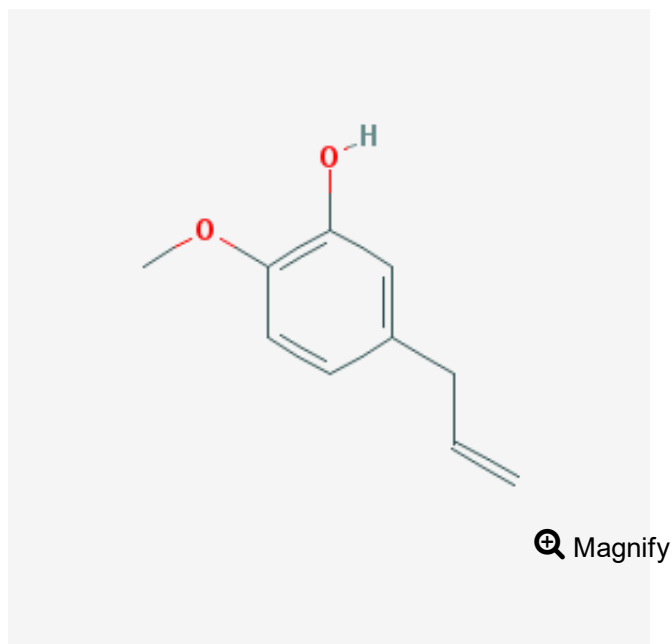
[11 Information Sources](#)

1 2D Structure

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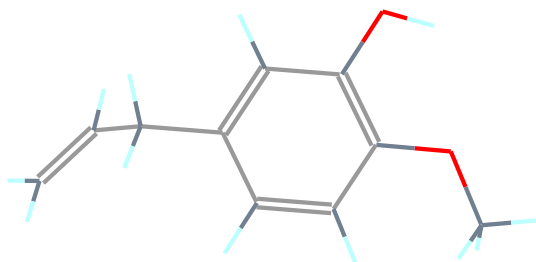
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2 3D Conformer

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 Magnify

Show Hydrogens

Show Atoms

Interact

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3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

2-methoxy-5-prop-2-enylphenol

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3.1.2 InChI

InChI=1S/C10H12O2/c1-3-4-8-5-6-10(12-2)9(11)7-8/h3,5-7,11H,1,4H2,2H3

▶ *from PubChem*

3.1.3 InChI Key

NPBVQXIMTZKSBA-UHFFFAOYSA-N

▶ *from PubChem*

3.1.4 Canonical SMILES

COC1=C(C=C(C=C1)CC=C)O

▶ *from PubChem*

3.2 Other Identifiers

3.2.1 UNII

OE7NQ16G4D

▶ *from FDA/SPL Indexing data*

3.2.2 Wikipedia

[Chavibetol](#)

▶ *from Wiki*

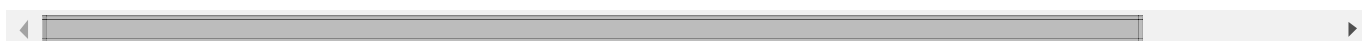
3.3 Synonyms

3.3.1 MeSH Synonyms

1. 5-allyl-2-methoxyphenol
2. chavibetol

3.3.2 Depositor-Supplied Synonyms

- | | | |
|---------------------------------------|------------------------------------|-----------------------|
| 1. Chavibetol | 11. UNII-OE7NQ16G4D | 21. BB_NC-0478 |
| 2. m-Eugenol | 12. 5-Allyl-2-methoxyphenol # | 22. BBL028696 |
| 3. 501-19-9 | 13. OE7NQ16G4D | 23. STL371291 |
| 4. Phenol, 5-allyl-2-methoxy- | 14. SCHEMBL901503 | 24. ZINC00517281 |
| 5. 2-methoxy-5-prop-2-enyl-phenol | 15. CHEMBL259093 | 25. AKOS006243252 |
| 6. 2-methoxy-5-(prop-2-en-1-yl)phenol | 16. 2-methoxy-5-prop-2-enylphenol | 26. Phenol, 2-methoxy |
| 7. meta-Eugenol | 17. CTK4J2176 | 27. 2-METHOXY-5-(1- |
| 8. AC1LC8RQ | 18. 2-Methoxy-5-(2-propenyl)phenol | 28. MCULE-218874601 |
| 9. 3-Allyl-6-methoxyphenol | 19. MolPort-002-507-060 | 29. KB-231206 |
| 10. 5-Allyl-2-methoxyphenol | 20. NPBVQXIMTZKSBA-UHFFFAOYSA-N | |



4 Chemical and Physical Properties

4.1 Computed Properties

Molecular Weight	164.20108 g/mol
Molecular Formula	C₁₀H₁₂O₂
XLogP3	2
Hydrogen Bond Donor Count	1
Hydrogen Bond Acceptor Count	2
Rotatable Bond Count	3
Exact Mass	164.08373 g/mol
Monoisotopic Mass	164.08373 g/mol
Topological Polar Surface Area	29.5 A ²
Heavy Atom Count	12
Formal Charge	0
Complexity	145
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	1

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5 Related Records

5.1 Related Compounds with Annotation

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5.2 Related Compounds

Same Tautomer	4 records
Same Parent, Tautomer	5 records
Same Parent, Exact	2 records
Mixtures, Components, and Neutralized Forms	2 records
Similar Compounds	3048 records
Similar Conformers	1627 records

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5.3 Related Substances

All	28 records
Same	26 records
Mixture	2 records

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6 Chemical Vendors

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Vendor/Supplier	Purchasable Chemical	PubChem SID
Mcule	MCULE-2188746063	166223232
Ambinter	BB_NC-0478	25621675
ZINC	ZINC00517281	1180594
ChemFrog	888-743-590	125688333
ChemMol	99115791	241106687
Vitas-M Laboratory	BBL028696	184015556
	STL371291	173894675
AKos Consulting & Solutions	AKOS006243252	132525879
Chembase.cn	119200	162103172
MolPort	MolPort-002-507-060	90451432
Chembo	KB-231206	172880664
ABI Chem	AC1LC8RQ	113498711

▶ *from PubChem*

7 Literature

7.1 NLM Curated PubMed Citations

[All NLM Curated PubMed Citations](#)


▶ *from PubChem*

8 Patents

8.1 Depositor-Supplied Patent Identifiers

▼ Refine/Analyze

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1 to 10 of 18 1 2  Relevance ▼

Patent	Submitted	Granted
Polypropylene resin-based films and sheets [US6245840]		2001-06-12
Polypropylene resin composition, and film and sheet using the same [US6284822]		2001-09-04
Polypropylene resin-based films and sheets [US6545069]	2001-09-27	2003-04-08
Polypropylene resin composition, and film and sheet using the same [US6545072]	2002-08-01	2003-04-08
Flexible polypropylene resin [US6855756]	2003-03-20	2005-02-15
DECORATIVE FILM OR SHEET, AND DECORATIVE MATERIAL AND BUILDING MATERIAL MADE BY USING THE SAME [EP0893247]	1999-01-27	2007-04-11
FLEXIBLE POLYPROPYLENE RESIN COMPOSITIONS, FILMS OR SHEETS MADE THEREFROM, AND SURFACE-PROTECTIVE FILMS OR SHEETS MADE THEREFROM [EP0927743]	1999-07-07	2003-03-19
Antimonocytic activity of betel leaf extracts [US2002068096]	2001-01-30	2002-06-06
ANTI-LEISHMANIAL ACTIVITY OF BETEL LEAF EXTRACT [US2002098251]	2001-01-30	2002-07-25
Use of betel leaf extract to induce IFN-gamma production from human peripheral blood T cells and as a Th1 type immunomodulator [US2006013900]	2005-09-12	2006-01-19

▶ from PubChem

9 Biological Test Results

9.1 BioAssay Results

 Refine/Analyze

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1 to 4 of 4 ◆ Relevance ▼

Activity	Substance	BioAssay
unspecified	103569181	Protection against 30 mins photoirradiation-induced damage in rat liver mitochondria assessed as reduction of lipid hydroperoxide formation at 180 uM [AID: 323189]
unspecified	103569181	Protection against 30 mins photoirradiation-induced lipid peroxidation damage in rat liver mitochondria assessed as prevention of TBARS formation at 180 uM [AID: 323188]
unspecified	103569181	Protection against 30 mins photoirradiation-induced lipid peroxidation damage in rat liver mitochondria assessed as prevention of TBARS formation at 60 uM [AID: 323187]
unspecified	103569181	Protection against 30 mins photoirradiation-induced lipid peroxidation damage in rat liver mitochondria assessed as prevention of TBARS formation at 30 uM [AID: 323186]

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10 Classification

10.1 Ontologies

10.1.1 MeSH Tree

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1 to 1 of 1

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chavibetol

[▶ from MeSH](#)

10.1.2 WIPO IPC

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1 to 10 of 128 **1** 2 3 ... 13
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A61P29/00 - Non-central analgesic, antipyretic or antiinflammatory agents, e.g. antirheuma...

A61P31/04 - Antibacterial agents

A61P31/20 - for DNA viruses

A61P35/00 - Antineoplastic agents

A61P35/02 - specific for leukemia

A61P43/00 - Drugs for specific purposes, not provided for in groups A61P1/00-A61P41/00

A61Q11/00 - Preparations for care of the teeth, of the oral cavity or of dentures, e.g. d...

A61Q13/00 - Formulations or additives for perfume preparations

A61Q15/00 - Anti-perspirants or body deodorants

C07D263/18 - Oxygen atoms

[▶ from WIPO](#)

10.2 Substance Categorization Classification

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➤ Biological Properties (6)

➤ Chemical Reactions (1)

➤ Database Vendor (1)

➤ Journal Publishers (1)

➤ Patents (3)

➤ Physical Properties (2)

▼ Substance Vendors (12)

▼ Refine/Analyze

Source	External ID	PubChem SID
Mcule	MCULE-2188746063	166223232
Ambinter	BB_NC-0478	25621675
ZINC	ZINC00517281	1180594
ChemFrog	888-743-590	125688333
ChemMol	99115791	241106687
Vitas-M Laboratory	BBL028696	184015556
	STL371291	173894675
AKos Consulting & Solutions	AKOS006243252	132525879
Chembase.cn	119200	162103172
MolPort	MolPort-002-507-060	90451432
Chembo	KB-231206	172880664
ABI Chem	AC1LC8RQ	113498711

▼ Theoretical Properties (4)

▼ Refine/Analyze

Source	External ID	PubChem SID
ChemDB	4554113	5183024
ChemSpider	518422	43156581
Mcule	MCULE-2188746063	166223232
ZINC	ZINC00517281	1180594

➤ Toxicology (1)

▶ from PubChem

11 Information Sources

1. Wiki 10009 <http://en.wikipedia.org/wiki/Chavibetol>
2. FDA/SPL Indexing data OE7NQ16G4D
<http://www.fda.gov/ForIndustry/DataStandards/StructuredProductLabeling/ucm377913.htm>
3. PubChem <http://pubchem.ncbi.nlm.nih.gov>
Data deposited in or computed by PubChem
4. chavibetol from MeSH 67542039 <http://www.ncbi.nlm.nih.gov/mesh/67542039>
5. MeSH Tree from MeSH DescTree <http://www.nlm.nih.gov/mesh/meshhome.html>
MeSH (Medical Subject Headings) is the NLM controlled vocabulary thesaurus used for indexing articles for PubMed.
6. International Patent Classification 2015 from WIPO IPC <http://www.wipo.int/classifications/ipc/>
The World Intellectual Property Organization (WIPO) International Patent Classification (IPC) provides for a hierarchical system of language independent symbols for the classification of patents and utility models according to the different areas of technology to which they pertain.