A

Ocimum tenuiflorum

Kingdom: Plantae

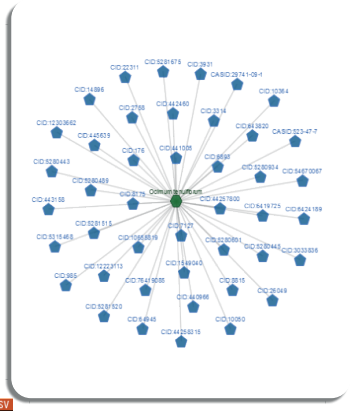
Family: Lamiaceae

More Information:

PlantList | Tropicos | FRLHT

INDIAN MEDICINAL PLANT	PHYTOCHEMICAL IDENTIFIER	PHYTOCHEMICAL NAME	REFERENCES
Ocimum tenuiflorum	CID:12303662	Phytosterols	ISBN:9788171360536
Ocimum tenuiflorum	CID:440966	(-)-camphene	ISBN:9788171360536
Ocimum tenuiflorum	CID:443158	(-)-Linalool	DOI:10.15482/USDA.ADC/1239279
Ocimum tenuiflorum	CID:441005	(+)-delta-Cadinene	DOI:10.15482/USDA.ADC/1239279
Ocimum tenuiflorum	CID:442460	(1S,2R,4S)-(-)-Bornyl acetate	ISBN:9788171360536
Ocimum tenuiflorum	CID:10050	(1S)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one	ISBN:9788171360536
Ocimum tenuiflorum	CID:5315468	(E)-alpha-bisabolene	DOI:10.15482/USDA.ADC/1239279
Ocimum tenuiflorum	CID:6424189	1-(4-Hydroxy-3-Methoxyphenyl)-1,2,3-Tris(4-Allyl-2-Methoxyphenoxy)Propane	DOI:10.15482/USDA.ADC/1239279

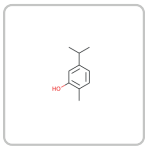
Cytoscape network of Indian Medicinal Plant and its known phytochemicals



CSV

B

CARVACROL



View 3D structure using JSmol

Download structure:

2D: 2D MOL | 2D MOL2 | 2D SDF

3D: 3D MOL | 3D MOL2 | 3D SDF | 3D PDB | 3D PDBQT

Chemical kingdom: Organic compounds

Superclass: Lipids and lipid-like molecules

Class: Prenol lipids

Subclass: Monoterpenoids

PubChem Identifier: 10364

ChEBI Identifier: 3440

CAS Identifier: 499-75-2

Synonyms: CARVACROL;ACETYLGITOXINS

Canonical SMILES: CC(c1ccc(c(c1)O)C)C

InChI Key: RECUKUPTGUEGMW-UHFFFAOYSA-N

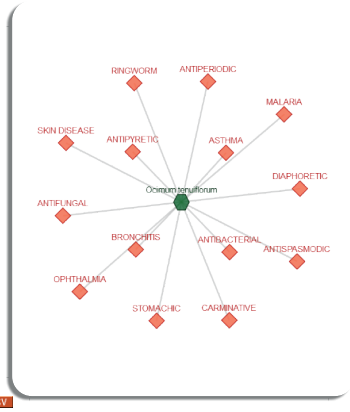
Physicochemical Properties

Property	Value
Molecular weight	150.22 g/mol
LogP	2.82
LogD	3.43
LogSw	-3.08
Number of stereocenters	0
Stereochemical complexity	0.000
Fsp3	0.400
Topological polar surface area	20.23 $Å^2$

C

INDIAN MEDICINAL PLANT	THERAPEUTIC USE	THERAPEUTIC IDENTIFIER	REFERENCES
Ocimum tenuiflorum	ANTIBACTERIAL		ISBN:978-0-387-70637-5
Ocimum tenuiflorum	ANTIFUNGAL	DOID:1564	ISBN:978-0-387-70637-5
Ocimum tenuiflorum	ANTIPERIODIC		ISBN:978-0-387-70637-5
Ocimum tenuiflorum	ANTIPYRETIC	DOID:11100	ISBN:978-0-387-70637-5
Ocimum tenuiflorum	ANTISPASMODIC		ISBN:978-0-387-70637-5
Ocimum tenuiflorum	ASTHMA	MESH:D001249,MESH:D001250,MESH:D016535 UMLS:C0004096, UMLS:C0004099, UMLS:C0085129, UMLS:C0155883 DOID:2841	ISBN:978-0-387-70637-5, ISBN:9788171360536
Ocimum tenuiflorum	BRONCHITIS	MESH:D001991, MESH:D029481 UMLS:C0006277, UMLS:C0008677, UMLS:C0149514, UMLS:C2939171 DOID:6132	ISBN:9788171360536

Cytoscape network of Indian Medicinal Plant and its therapeutic uses



CSV

D

Physicochemical properties | Drug-like filters | Chemical similarity filter

Molecular weight (g/mol) Is equal to

LogP Is equal to

Topological polar surface area ($Å^2$) Is equal to

Number of hydrogen bond acceptor Is equal to

Number of hydrogen bond donors Is equal to

Number of heavy atoms Is equal to

Number of heteroatoms Is equal to

Number of rigid bonds Is equal to

Number of rotatable bonds Is equal to

Stereochemical complexity Is equal to

Fsp3 Is equal to

Apply

Select any filter and click on Apply to see results

Physicochemical properties | Drug-like filters | Chemical similarity filter

Lipinski RO5 violation - Any -

Oral PhysChem score - Any -

GSK 4/400 - Any -

Pfizer 3/75 - Any -

Veber rule - Any -

Egan rule - Any -

QEDw Is equal to

Apply

Select any filter and click on Apply to see results

Physicochemical properties | Drug-like filters | Chemical similarity filter

Enter SMILES *

Choose Fingerprint *

- Select -

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