Compound Summary for CID 3198

Econazole

Cite this Record

STRUCTURE VENDORS DRUG INFO PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID:	3198
Chemical Names:	Econazole; Ecostatin; 27220-47-9; Pevaryl; Gyno-pevaryl; Econazolum More...
Molecular Formula:	$C_{18}H_{15}Cl_3N_2O$
Molecular Weight:	381.681 g/mol
InChI Key:	LEZWWPYKPKIXLL-UHFFFAOYSA-N
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)
Drug Information:	Drug Indication FDA Orange Book

Econazole is an imidazole derivative that is commonly used as a topical antifungal agent.

from MeSH

Econazole is only found in individuals that have used or taken this drug. It is a broad spectrum antimycotic with some action against Gram positive bacteria. It is used topically in dermatomycoses also orally and parenterally. [PubChem]Econazole interacts with 14-alpha demethylase, a cytochrome P-450 enzyme necessary to convert lanosterol to ergosterol. As ergosterol is an essential component of the fungal cell membrane, inhibition of its synthesis results in increased cellular permeability causing leakage of cellular contents. Econazole may also inhibit endogenous respiration, interact with membrane phospholipids, inhibit the transformation of yeasts to mycelial forms, inhibit purine uptake, and impair triglyceride and/or phospholipid biosynthesis.

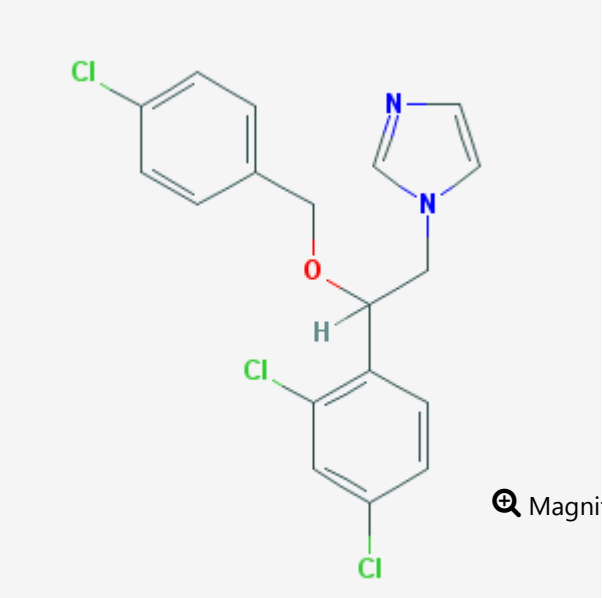
Metabolite Description from Human Metabolome Database

PUBCHEM > COMPOUND > ECONAZOLE *Create Date: 2005-03-25*

Contents

1 2D Structure

Search Download Get Image



Magnify

from PubChem

2 3D Conformer

Search Download Get Image

CLICK TO LOAD...

Magnify

Show Hydrogens Show Atoms Animate

from PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

1-[2-[(4-chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]imidazole

from PubChem

3.1.2 InChI

InChI=1S/C18H15Cl3N2O/c19-14-3-1-13(2-4-14)11-24-18(10-23-8-7-22-12-23)16-6-5-15(20)9-17(16)21/h1-9,12,18H,10-11H2

from PubChem

3.1.3 InChI Key

LEZWWPYKPKIXLL-UHFFFAOYSA-N

from PubChem

3.1.4 Canonical SMILES

C1=CC(=CC=C1COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl)Cl

from PubChem

3.2 Molecular Formula

$C_{18}H_{15}Cl_3N_2O$

from PubChem

3.3 Other Identifiers

3.3.1 CAS

27220-47-9

from ChemIDplus, DrugBank, European Chemicals Agency - ECHA, Human Metabolome Database

68797-30-8

DOCKET ALARM

Explore Litigation Insights

Docket Alarm provides insights to develop a more informed litigation strategy and the peace of mind of knowing you're on top of things.

Real-Time Litigation Alerts

Keep your litigation team up-to-date with **real-time alerts** and advanced team management tools built for the enterprise, all while greatly reducing PACER spend.

Our comprehensive service means we can handle Federal, State, and Administrative courts across the country.

Advanced Docket Research

With over 230 million records, Docket Alarm's cloud-native docket research platform finds what other services can't. Coverage includes Federal, State, plus PTAB, TTAB, ITC and NLRB decisions, all in one place.

Identify arguments that have been successful in the past with full text, pinpoint searching. Link to case law cited within any court document via Fastcase.

Analytics At Your Fingertips

Learn what happened the last time a particular judge, opposing counsel or company faced cases similar to yours.

Advanced out-of-the-box PTAB and TTAB analytics are always at your fingertips.

API

Docket Alarm offers a powerful API (application programming interface) to developers that want to integrate case filings into their apps.

LAW FIRMS
Build custom dashboards for your attorneys and clients with live data direct from the court.

Automate many repetitive legal tasks like conflict checks, document management, and marketing.

FINANCIAL INSTITUTIONS
Litigation and bankruptcy checks for companies and debtors.

E-DISCOVERY AND LEGAL VENDORS
Sync your system to PACER to automate legal marketing.