

Itraconazole

Cat. No.:	OB0225LY-0248
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, HPLC, and LC-MS.
Size:	50 mg; 100 mg; 200 mg; 500 mg

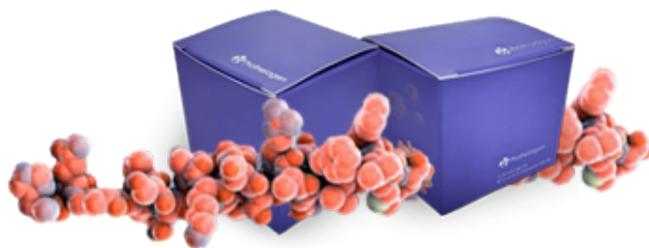
This product is for research use only and is not intended for diagnostic use.

Product Overview

Description	Itraconazole is a triazole antifungal agent that inhibits cytochrome P-450-dependent enzymes.
Synonym	R51211; 84625-61-6; Sporanox; Oriconazole; Itraconazol; Itrizole; 2-Butan-2-yl-4-[4-[4-[[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1,2,4-triazol-1-yl)methyl]-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]phenyl]-1,2,4-triazol-3-one; 1-(Butan-2-yl)-4-[4-[4-[[[(2R,4S)-2-(2,4-dichlorophenyl)-2-[(1H-1,2,4-triazol-1-yl)methyl]-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]phenyl]-4,5-dihydro-1H-1,2,4-triazol-5-one; 3H-1,2,4-Triazol-3-one, 4-[4-[4-[[2-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)methyl]-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-2,4-dihydro-2-(1-methylpropyl); 4-[4-[4-[[[(2R,4S)-2-(2,4-Dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)methyl]-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-2,4-dihydro-2-(1-methylpropyl)-3H-1,2,4-triazol-3-one
CAS No.	84625-61-6
Compound CID	55283
Formula	C ₃₅ H ₃₈ Cl ₂ N ₈ O ₄
Formula Weight	705.63

Specification

Relative Density	1.4 g/cm ³
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IUPAC Name	2-Butan-2-yl-4-[4-[4-[4-[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]phenyl]-1,2,4-triazol-3-one
InChI	InChI=1S/C35H38Cl2N8O4/c1-3-25(2)45-34(46)44(24-40-45)29-7-5-27(6-8-29)41-14-16-42(17-15-41)28-9-11-30(12-10-28)47-19-31-20-48-35(49-31,21-43-23-38-22-39-43)32-13-4-26(36)18-33(32)37/h4-13,18,22-25,31H,3,14-17,19-21H2,1-2H3/t25?,31-,35-/m0/s1
InChI Key	VHVPQPYKVGDNFY-ZPGVKDDISA-N
SMILES string	<chem>CCC(C)N1C(=O)N(C=N1)C2=CC=C(C=C2)N3CCN(CC3)C4=CC=C(C=C4)OC[C@H]5CO[C@](O5)(CN6C=NC=N6)C7=C(C=C(C=C7)Cl)Cl</chem>
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	Itraconazole can be used in microbiological studies to assess its inhibitory effect on fungal growth.

Library Information

Targets	P450; Hedgehog/Smoothened
Receptors	CYP3A4; Cytochrome P450
Pathways	Metabolism; GPCR/G protein; Autophagy; Stem cells; Microbiology/Virology
Plate Number	AOCL-4
Plate Location	b3
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	2 mM DMSO
DMSO Max Solubility	7.06 mg/mL; 10 mM
Solubility	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 0.71 mg/mL (1.01 mM)
ALogP	6.434
HBA_Count	7
HBD_Count	0
Rotatable Bond	11