

# Itraconazole

<b>Other names:</b>	4-(4-(4-(4-((2-((1H-1,2,4-triazol-1-yl)methyl)-2-(2,4-dichlorophenyl)-1,3-dioxolan-4-yl)methyl)ethyl)butyl)butyl)butyl)butyl)butyl Orungal
<b>Inchi:</b>	InChI=1S/C35H38Cl2N8O4/c1-3-25(2)45-34(46)44(24-40-45)29-7-5-27(6-8-29)41-14-16
<b>InchiKey:</b>	VHVPQPYKVGDNFY-UHFFFAOYSA-N
<b>Formula:</b>	C35H38Cl2N8O4
<b>SMILES:</b>	CCC(C)n1ncn(-c2ccc(N3CCN(c4ccc(OCC5COC(Cn6cncn6)(c6ccc(Cl)cc6Cl)O5)cc4)CC3
<b>Mol. weight [g/mol]:</b>	705.65

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.96		Crippen Method
logp	5.577		Crippen Method
mcvol	499.890	ml/mol	McGowan Method
tt	362.15	K	A SAXS-WAXS study of the endothermic transitions in amorphous or supercooled liquid itraconazole
tt	346.85	K	A SAXS-WAXS study of the endothermic transitions in amorphous or supercooled liquid itraconazole

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>A SAXS-WAXS study of the endothermic transitions in amorphous or supercooled liquid itraconazole:</b>	<a href="https://www.doi.org/10.1016/j.tca.2016.10.004">https://www.doi.org/10.1016/j.tca.2016.10.004</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tt:** Triple Point Temperature

Latest version available from:

<https://www.cheméo.com/cid/109-230-5/Itraconazole.pdf>

Generated by Cheméo on 2024-08-18 10:44:37.645867318 +0000 UTC m=+2667746.892972678.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.