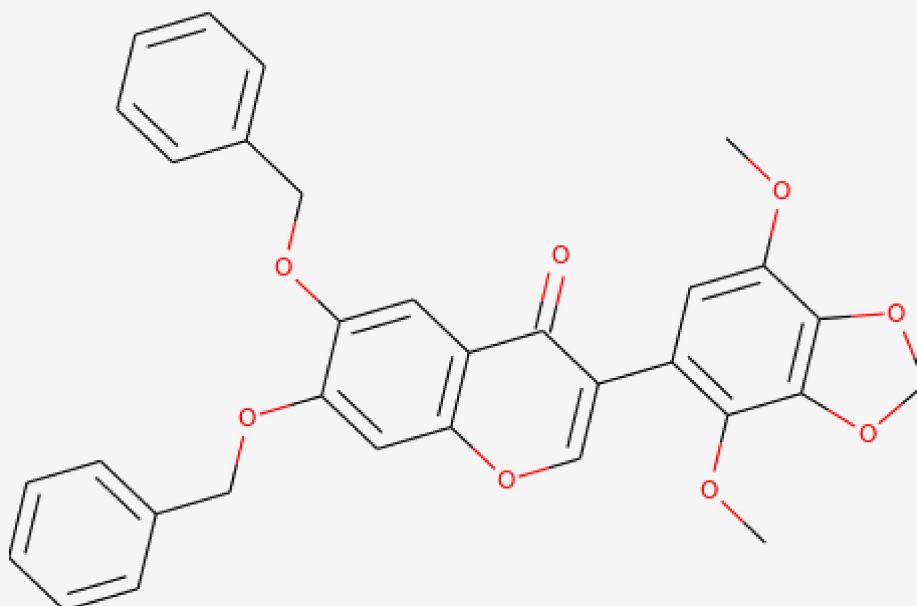


# Pharmacokinetic Properties

## Molecule Depiction

[SMILES](#)

## Molecule properties:

Descriptor	Value
Molecular Weight	538.552
LogP	6.3639
#Rotatable Bonds	9
#Acceptors	8
#Donors	0
Surface Area	229.751

Property	Model Name	Predicted Value	Unit

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	-3.606	Numeric (log mol/L)
Absorption	Caco2 permeability	1.15	Numeric (log Papp in 10 <sup>-6</sup> cm/s)
Absorption	Intestinal absorption (human)	97.127	Numeric (% Absorbed)
Absorption	Skin Permeability	-2.735	Numeric (log Kp)
Absorption	P-glycoprotein substrate	No	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	Yes	Categorical (Yes/No)
Distribution	VDss (human)	-1.023	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.356	Numeric (Fu)
Distribution	BBB permeability	-1.232	Numeric (log BB)
Distribution	CNS permeability	-2.787	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	Yes	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	Yes	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	Yes	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	Yes	Categorical (Yes/No)
Excretion	Total Clearance	0.337	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	No	Categorical (Yes/No)
Toxicity	AMES toxicity	No	Categorical (Yes/No)
Toxicity	Max. tolerated dose (human)	0.613	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	No	Categorical (Yes/No)
Toxicity	hERG II inhibitor	Yes	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	2.925	Numeric (mol/kg)

Property	Model Name	Predicted Value	Unit
<b>Toxicity</b>	Oral Rat Chronic Toxicity (LOAEL)	<b>0.481</b>	Numeric (log mg/kg_bw/day)
<b>Toxicity</b>	Hepatotoxicity	<b>Yes</b>	Categorical (Yes/No)
<b>Toxicity</b>	Skin Sensitisation	<b>No</b>	Categorical (Yes/No)
<b>Toxicity</b>	<i>T.Pyriformis</i> toxicity	<b>0.285</b>	Numeric (log ug/L)
<b>Toxicity</b>	Minnow toxicity	<b>-2.401</b>	Numeric (log mM)

Run another prediction

Back



Best viewed using [Chrome](#) on 1280x1024 resolution and above

