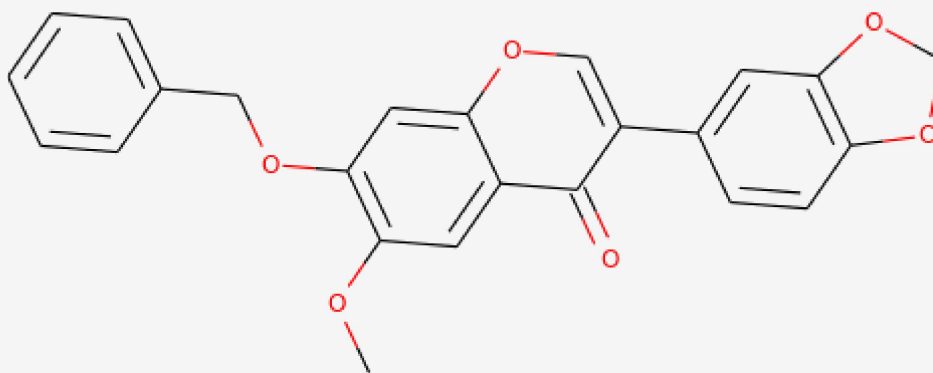


# Pharmacokinetic Properties

## Molecule Depiction

[SMILES](#)

## Molecule properties:

Descriptor	Value
Molecular Weight	402.402
LogP	4.7763
#Rotatable Bonds	5
#Acceptors	6
#Donors	0
Surface Area	171.737

Property	Model Name	Predicted Value	Unit
<b>Absorption</b>	Water solubility	<b>-3.993</b>	Numeric (log mol/L)
<b>Absorption</b>	Caco2 permeability	<b>1.157</b>	Numeric (log Papp in 10 <sup>-6</sup> cm/s)

Property	Model Name	Predicted Value	Unit
Absorption	Intestinal absorption (human)	99.169	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)	-0.335	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.263	Numeric (Fu)
Distribution	BBB permeability	-0.111	Numeric (log BB)
Distribution	CNS permeability	-2.052	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	Yes	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	Yes	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	0.249	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)	0.739	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)	2.768	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	0.917	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	No	Categorical (Yes/No)
Toxicity	Skin Sensitisation	No	Categorical (Yes/No)

Property	Model Name	Predicted Value	Unit
Toxicity	<i>T.Pyriformis</i> toxicity	0.286	Numeric (log ug/L)
Toxicity	Minnow toxicity	-1.364	Numeric (log mM)

Run another prediction

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