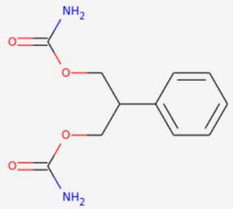
Molecule Depiction



SMILES

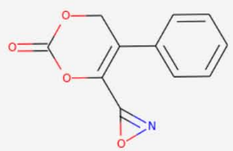
Molecule properties:

Descriptor	Value
Molecular Weight	238.243
LogP	0.9608
#Rotatable Bonds	5
#Acceptors	4
#Donors	2
Surface Area	98.486

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	**-1.609**	Numeric (log mol/L)
Absorption	Caco2 permeability	**0.121**	Numeric (log Papp in 10^{-6} cm/s)
Absorption	Intestinal absorption (human)	**67.854**	Numeric (% Absorbed)
Absorption	Skin Permeability	**-3.143**	Numeric (log Kp)
Absorption	P-glycoprotein substrate	**No**	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	**No**	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	**No**	Categorical (Yes/No)
Distribution	VDss (human)	**-0.299**	Numeric (log L/kg)
Distribution	Fraction unbound (human)	**0.459**	Numeric (Fu)
Distribution	BBB permeability	**-0.206**	Numeric (log BB)
Distribution	CNS permeability	**-2.87**	Numeric (log PS)
Metabolism	CYP2D6 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitior	**No**	Categorical (Yes/No)
Excretion	Total Clearance	**0.265**	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)	**1.173**	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	**No**	Categorical (Yes/No)
Toxicity	hERG II inhibitor	**No**	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	**2.545**	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	**1.941**	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	**Yes**	Categorical (Yes/No)
Toxicity	Skin Sensitisation	**No**	Categorical (Yes/No)
Toxicity	*T.Pyriformis* toxicity	**0.542**	Numeric (log ug/L)
Toxicity	Minnow toxicity	**2.037**	Numeric (log mM)

Run another prediction Back

Molecule Depiction



SMILES

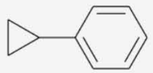
Molecule properties:

Descriptor	Value
Molecular Weight	217.18
LogP	1.9082
#Rotatable Bonds	2
#Acceptors	5
#Donors	0
Surface Area	90.906

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	**-2.02**	Numeric (log mol/L)
Absorption	Caco2 permeability	**1.269**	Numeric (log Papp in 10^{-6} cm/s)
Absorption	Intestinal absorption (human)	**95.615**	Numeric (% Absorbed)
Absorption	Skin Permeability	**-2.968**	Numeric (log Kp)
Absorption	P-glycoprotein substrate	**No**	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	**No**	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	**No**	Categorical (Yes/No)
Distribution	VDss (human)	**-0.107**	Numeric (log L/kg)
Distribution	Fraction unbound (human)	**0.298**	Numeric (Fu)
Distribution	BBB permeability	**-0.125**	Numeric (log BB)
Distribution	CNS permeability	**-2.358**	Numeric (log PS)
Metabolism	CYP2D6 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	**Yes**	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitior	**Yes**	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitior	**No**	Categorical (Yes/No)
Excretion	Total Clearance	**0.369**	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	**No**	Categorical (Yes/No)
Toxicity	AMES toxicity	**Yes**	Categorical (Yes/No)
Toxicity	Max. tolerated dose (human)	**0.379**	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	**No**	Categorical (Yes/No)
Toxicity	hERG II inhibitor	**No**	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	**2.445**	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	**1.842**	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	**No**	Categorical (Yes/No)
Toxicity	Skin Sensitisation	**No**	Categorical (Yes/No)
Toxicity	*T.Pyriformis* toxicity	**0.939**	Numeric (log ug/L)
Toxicity	Minnow toxicity	**1.325**	Numeric (log mM)

Run another prediction | Back

Molecule Depiction



SMILES

Molecule properties:

Descriptor	Value
Molecular Weight	118.179
LogP	2.564
#Rotatable Bonds	1
#Acceptors	0
#Donors	0
Surface Area	55.520

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	**-3.59**	Numeric (log mol/L)
Absorption	Caco2 permeability	**1.499**	Numeric (log Papp in 10^{-6} cm/s)
Absorption	Intestinal absorption (human)	**96.105**	Numeric (% Absorbed)
Absorption	Skin Permeability	**-1.148**	Numeric (log Kp)
Absorption	P-glycoprotein substrate	**No**	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	**No**	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	**No**	Categorical (Yes/No)
Distribution	VDss (human)	**0.611**	Numeric (log L/kg)
Distribution	Fraction unbound (human)	**0.287**	Numeric (Fu)
Distribution	BBB permeability	**0.516**	Numeric (log BB)
Distribution	CNS permeability	**-1.394**	Numeric (log PS)
Metabolism	CYP2D6 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitior	**Yes**	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitior	**No**	Categorical (Yes/No)
Excretion	Total Clearance	**0.146**	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)	**0.642**	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	**No**	Categorical (Yes/No)
Toxicity	hERG II inhibitor	**No**	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	**1.718**	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	**2.305**	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	**No**	Categorical (Yes/No)
Toxicity	Skin Sensitisation	**Yes**	Categorical (Yes/No)
Toxicity	*T.Pyriformis* toxicity	**0.914**	Numeric (log ug/L)
Toxicity	Minnow toxicity	**0.981**	Numeric (log mM)

Run another prediction Back

Toxtree (Estimation of Toxic Hazard - A Decision Tree Approach) v3.1.0-1851-1525442531402

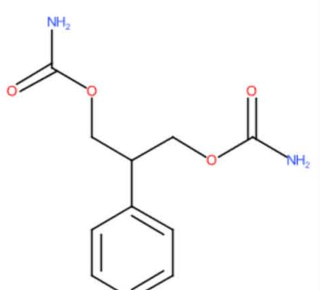
File Edit Chemical Compounds Toxic Hazard Method Help

« » Chemical identifier O=C(N)OCC(COC(N)=O)C1=CC=CC=C1 Go!

Available structure attributes

Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	NO
Negative for nongenoto...	YES
Potential S. typhimurium ...	NO
Potential carcinogen bas...	NO
QSAR6,8 applicable?	NO
SA10_gen	NO
SA11_gen	NO
SA12_gen	NO
SA13_gen	NO

Structure diagram



First Prev 1 / 1 Next Last

Toxic Hazard by Carcinogenicity (genotox and nongenotox) and mutagenicity rulebase by ISS

Estimate

Structural Alert for genotoxic carcinogenicity

Structural Alert for nongenotoxic carcinogenicity

Potential S. typhimurium TA100 mutagen based on QSAR

Unlikely to be a S. typhimurium TA100 mutagen based on QSAR

☑ Verbose explanation

Carcinogenicity (genotox and nongenotox) and mutagenicity rulebase by ISS

Decision method has not been applied yet!

Type here to search

27°C Light rain ENG 19:36 23-08-2021

Toxtree (Estimation of Toxic Hazard - A Decision Tree Approach) v3.1.0-1851-1525442531402

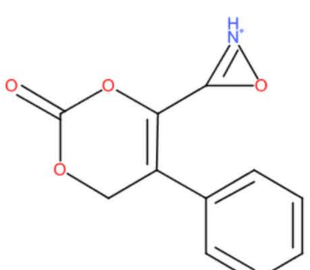
File Edit Chemical Compounds Toxic Hazard Method Help

« » Chemical identifier O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3 Go!

Available structure attributes

Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
Potential S. typhimurium ...	NO
Potential carcinogen bas...	NO
QSAR13 applicable?	NO
QSAR6,8 applicable?	NO
SA10_gen	NO
SA11_gen	NO
SA12_gen	NO

Structure diagram



First Prev 1 / 1 Next Last

Toxic Hazard by Carcinogenicity (genotox and nongenotox) and mutagenicity rulebase by ISS

Estimate

Structural Alert for genotoxic carcinogenicity

Structural Alert for nongenotoxic carcinogenicity

Potential S. typhimurium TA100 mutagen based on QSAR

Unlikely to be a S. typhimurium TA100 mutagen based on QSAR

Verbose explanation

Assigned according to the output of QSAR6 or QSAR13

Carcinogenicity (genotox and nongenotox) and mutagenicity rulebase by ISS

QSA1_gen.Acyl halides No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA3_gen.N-methylol derivatives No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA4_gen.Monohaloalkene No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA5_gen.S or N mustard No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA6_gen.Propiolactones and propiosultones No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA7_gen.Epoxides and aziridines No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA8_gen.Aliphatic halogens No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA9_gen.Alkyl nitrite No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA11_gen.Simple aldehyde No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA12_gen.Quinones No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA13_gen.Hydrazine No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA14_gen.Aliphatic azo and azoxy No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA15_gen.Isocyanate and isothiocyanate groups No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA16_gen.Alkyl carbamate and thiocarbamate No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA18_gen.Polycyclic Aromatic Hydrocarbons No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA19_gen.Heterocyclic Polycyclic Aromatic Hydrocarbons No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA21_gen.Alkyl and aryl N-nitroso groups No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA22_gen.Azide and triazene groups No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA23_gen.Aliphatic N-nitro No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA24_gen.α,β unsaturated alkoxy No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA25_gen.Aromatic nitroso group No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA26_gen.Aromatic ring N-oxide No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA27_gen.Nitro aromatic No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA28_gen.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA28bis_gen.Aromatic mono- and dialkylamine No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA28ter_gen.Aromatic N-acyl amine No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA29_gen.Aromatic diazo No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA30_gen.Coumarins and Furocoumarins No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA37_gen.Pyrrolizidine Alkaloids No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA38_gen.Alkenylbenzenes No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA39_gen_and_nogen.Steroidal estrogens No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QGenotoxic alert?.At least one alert for genotoxic carcinogenicity fired? No Class Negative for genotoxic carcinogenicity O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QQSAR13 applicable?.α,β unsaturated aldehyde No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA10_gen.α,β unsaturated carbonyls No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QaN=Na.Aromatic diazo No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

Qar-N=CH2.Derived aromatic amines No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QQSAR6,8 applicable?.Aromatic amine without sulfonic group on the same ring No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

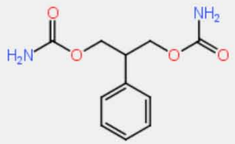
QSA17_nogen.Thiocarbonyl (Nongenotoxic carcinogens) No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA20_nogen.(Poly) Halogenated Cycloalkanes (Nongenotoxic carcinogens) No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

QSA31a_nogen.Halogenated benzene (Nongenotoxic carcinogens) No O=C(OC1)OC(C2=[NH+]O2)=C1C3=CC=CC=C3

Completed.

Enter compound name, SMILES or CAS-no: O=C(N)OCC(COC(N)=O)C1=CC=CC=C1



Toxicity Risks

- mutagenic
- tumorigenic
- irritant
- reproductive effective

cLogP 0.72

Solubility -2.82

Molweight 238.0

TPSA 104.6

Druglikeness 2.03

Drug-Score 0.87

Help

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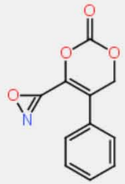
23-08-2021

Enter compound name, SMILES or CAS-no: O=C(OC1)OC(C2=NO2)=C1C3=CC=CC=C3



Toxicity Risks

- mutagenic
- tumorigenic
- irritant
- reproductive effective

cLogP 1.6

Solubility -2.96

Molweight 217.0

TPSA 60.42

Druglikeness -0.98

Drug-Score 0.58

Help

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19:42

23-08-2021