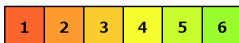


# Oral toxicity prediction results for input compound



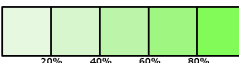
Predicted LD50: 810mg/kg

Predicted Toxicity Class: 4



Average similarity: 100%

Prediction accuracy: 100%



Name	CCC1=CC=CC=C1
Molweight	106.17
Number of hydrogen bond acceptors	0
Number of hydrogen bond donors	0
Number of atoms	8
Number of bonds	8
Number of rotatable bonds	1
Molecular refractivity	36.22
Topological Polar Surface Area	0
octanol/water partition coefficient(logP)	2.25

## Toxicity Model Report

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Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	<u>Hepatotoxicity</u>	dili	Inactive	0.86
Organ toxicity	<u>Neurotoxicity</u>	neuro	Active	0.58
Organ toxicity	<u>Nephrotoxicity</u>	nephro	Inactive	0.84
Organ toxicity	<u>Respiratory toxicity</u>	respi	Inactive	0.87
Organ toxicity	<u>Cardiotoxicity</u>	cardio	Inactive	0.65
Toxicity end points	<u>Carcinogenicity</u>	carcino	Active	0.89
Toxicity end points	<u>Immunotoxicity</u>	immuno	Inactive	0.99
Toxicity end points	<u>Mutagenicity</u>	mutagen	Inactive	0.98
Toxicity end points	<u>Cytotoxicity</u>	cyto	Inactive	0.91
Toxicity end points	<u>BBB-barrier</u>	bbb	Active	0.99
Toxicity end points	<u>Ecotoxicity</u>	eco	Active	0.81
Toxicity end points	<u>Clinical toxicity</u>	clinical	Inactive	0.80
Toxicity end points	<u>Nutritional toxicity</u>	nutri	Inactive	0.87
Tox21-Nuclear receptor signalling pathways	<u>Aryl hydrocarbon Receptor (AhR)</u>	nr_ahr	Inactive	1.0
Tox21-Nuclear receptor signalling pathways	<u>Androgen Receptor (AR)</u>	nr_ar	Inactive	1.0
Tox21-Nuclear receptor signalling pathways	<u>Androgen Receptor Ligand Binding Domain (AR-LBD)</u>	nr_ar_lbd	Inactive	0.99
Tox21-Nuclear receptor signalling pathways	<u>Aromatase</u>	nr_aromatase	Inactive	1.0
Tox21-Nuclear receptor signalling pathways	<u>Estrogen Receptor Alpha (ER)</u>	nr_er	Inactive	0.98
Tox21-Nuclear receptor signalling pathways	<u>Estrogen Receptor Ligand Binding Domain (ER-LBD)</u>	nr_er_lbd	Inactive	0.99
Tox21-Nuclear receptor signalling pathways	<u>Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)</u>	nr_ppar_gamma	Inactive	1.0
Tox21-Stress response pathways	<u>Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)</u>	sr_are	Inactive	1.0
Tox21-Stress response pathways	<u>Heat shock factor response element (HSE)</u>	sr_hse	Inactive	1.0
Tox21-Stress response pathways	<u>Mitochondrial Membrane Potential (MMP)</u>	sr_mmp	Inactive	1.0
Tox21-Stress response pathways	<u>Phosphoprotein (Tumor Suppressor) p53</u>	sr_p53	Inactive	1.0
Tox21-Stress response pathways	<u>ATPase family AAA domain-containing protein 5 (ATAD5)</u>	sr_atad5	Inactive	1.0
Molecular Initiating Events	<u>Thyroid hormone receptor alpha (THRα)</u>	mie_thr_alpha	Inactive	0.90
Molecular Initiating Events	<u>Thyroid hormone receptor beta (THRβ)</u>	mie_thr_beta	Inactive	0.78
Molecular Initiating Events	<u>Transthyretin (TTR)</u>	mie_ttr	Inactive	0.97
Molecular Initiating Events	<u>Ryanodine receptor (RYR)</u>	mie_ryr	Inactive	0.98
Molecular Initiating Events	<u>GABA receptor (GABAR)</u>	mie_gabar	Inactive	0.96
Molecular Initiating Events	<u>Glutamate N-methyl-D-aspartate receptor (NMDAR)</u>	mie_nmdar	Inactive	0.92
Molecular Initiating Events	<u>alpha-amino-3-hydroxy-5-methyl-4-isoxazolepropionate receptor (AMPA)</u>	mie_ampar	Inactive	0.97
Molecular Initiating Events	<u>Kainate receptor (KAR)</u>	mie_kar	Inactive	0.99
Molecular Initiating Events	<u>Achetylcholinesterase (AChE)</u>	mie_ache	Inactive	0.86
Molecular Initiating Events	<u>Constitutive androstane receptor (CAR)</u>	mie_car	Inactive	0.98
Molecular Initiating Events	<u>Pregnane X receptor (PXR)</u>	mie_pxr	Inactive	0.92
Molecular Initiating Events	<u>NADH-quinone oxidoreductase (NADHOX)</u>	mie_nadhox	Inactive	0.97
Molecular Initiating Events	<u>Voltage gated sodium channel (VGSC)</u>	mie_vgsc	Inactive	0.95

