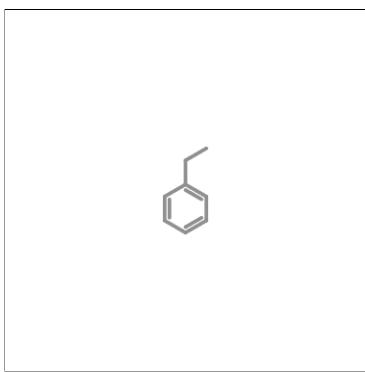
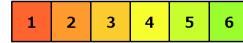


## Oral toxicity prediction results for input compound



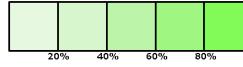
**Predicted LD50: 810mg/kg**

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

Classification	Target	Shorthand	Prediction	Probability
Molecular Initiating Events	<u>Na<sup>+</sup>/I<sup>-</sup> symporter (NIS)</u>	mie_nis	Inactive	0.98
Metabolism	<u>Cytochrome CYP1A2</u>	CYP1A2	Inactive	0.69
Metabolism	<u>Cytochrome CYP2C19</u>	CYP2C19	Inactive	0.61
Metabolism	<u>Cytochrome CYP2C9</u>	CYP2C9	Active	0.65
Metabolism	<u>Cytochrome CYP2D6</u>	CYP2D6	Inactive	0.71
Metabolism	<u>Cytochrome CYP3A4</u>	CYP3A4	Inactive	0.98
Metabolism	<u>Cytochrome CYP2E1</u>	CYP2E1	Inactive	0.92

## Toxicity targets

Possible binding to toxicity targets is shown below. For more information on the targets, please click on the individual abbreviations.



AA2AR ADRB2 ANDR AOFA CRFR1 DRD3 ESR1 ESR2 GCR HRH1 NR1I2 OPRK OPRM PDE4D PGH1 PRGR