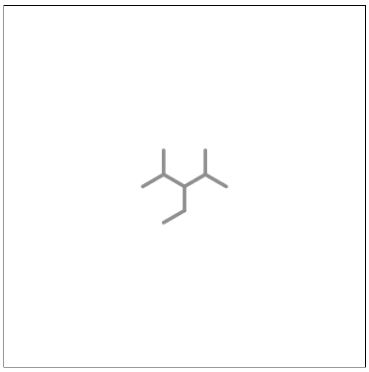
Oral toxicity prediction results for input compound



Predicted LD50: 2000mg/kg

Predicted Toxicity Class: 4

1 2 3 4 5 6

Average similarity: 100%

Prediction accuracy: 100%

20% 40% 60% 80%

Name	CCC(C(C)C)C(C)C
Molweight	128.26
Number of hydrogen bond acceptors	0
Number of hydrogen bond donors	0
Number of atoms	9
Number of bonds	8
Number of rotable bonds	3
Molecular refractivity	45.38
Topological Polar Surface Area	0
octanol/water partition coefficient(logP)	3.32

Toxicity Model Report

Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Calculating...	Calculating...
Organ toxicity	Neurotoxicity	neuro	Calculating...	Calculating...
Organ toxicity	Nephrotoxicity	nephro	Calculating...	Calculating...
Organ toxicity	Respiratory toxicity	respi	Calculating...	Calculating...
Organ toxicity	Cardiotoxicity	cardio	Calculating...	Calculating...
Toxicity end points	Carcinogenicity	carcino	Calculating...	Calculating...
Toxicity end points	Immunotoxicity	immuno	Calculating...	Calculating...
Toxicity end points	Mutagenicity	mutagen	Calculating...	Calculating...
Toxicity end points	Cytotoxicity	cyto	Calculating...	Calculating...
Toxicity end points	BBB-barrier	bbb	Calculating...	Calculating...
Toxicity end points	Ecotoxicity	eco	Calculating...	Calculating...
Toxicity end points	Clinical toxicity	clinical	Calculating...	Calculating...
Toxicity end points	Nutritional toxicity	nutri	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Aryl hydrocarbon Receptor (AhR)	nr_ahr	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Androgen Receptor (AR)	nr_ar	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	nr_ar_lbd	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Aromatase	nr_aromatase	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Alpha (ER)	nr_er	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	nr_er_lbd	Calculating...	Calculating...
Tox21-Nuclear receptor signalling pathways	Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)	nr_ppar_gamma	Calculating...	Calculating...
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	sr_are	Calculating...	Calculating...
Tox21-Stress response pathways	Heat shock factor response element (HSE)	sr_hse	Calculating...	Calculating...
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	sr_mmp	Calculating...	Calculating...
Tox21-Stress response pathways	Phosphoprotein (Tumor Supressor) p53	sr_p53	Calculating...	Calculating...
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	sr_atad5	Calculating...	Calculating...
Molecular Initiating Events	Thyroid hormone receptor alpha (THRα)	mie_thr_alpha	Calculating...	Calculating...
Molecular Initiating Events	Thyroid hormone receptor beta (THRβ)	mie_thr_beta	Calculating...	Calculating...
Molecular Initiating Events	Transtyretrin (TTR)	mie_ttr	Calculating...	Calculating...
Molecular Initiating Events	Ryanodine receptor (RYR)	mie_ryr	Calculating...	Calculating...
Molecular Initiating Events	GABA receptor (GABAR)	mie_gabar	Calculating...	Calculating...
Molecular Initiating Events	Glutamate N-methyl-D-aspartate receptor (NMDAR)	mie_nmdar	Calculating...	Calculating...
Molecular Initiating Events	alpha-amino-3-hydroxy-5-methyl-4-isoxazolepropionate receptor (AMPAR)	mie_ampar	Calculating...	Calculating...
Molecular Initiating Events	Kainate receptor (KAR)	mie_kar	Calculating...	Calculating...
Molecular Initiating Events	Achetylcholinesterase (AChE)	mie_ache	Calculating...	Calculating...
Molecular Initiating Events	Constitutive androstane receptor (CAR)	mie_car	Calculating...	Calculating...
Molecular Initiating Events	Pregnane X receptor (PXR)	mie_pxr	Calculating...	Calculating...
Molecular Initiating Events	NADH-quinone oxidoreductase (NADHOX)	mie_nadhox	Calculating...	Calculating...
Molecular Initiating Events	Voltage gated sodium channel (VGSC)	mie_vgsc	Calculating...	Calculating...
Molecular Initiating Events	Na+/I- symporter (NIS)	mie_nis	Calculating...	Calculating...
Metabolism	Cytochrome CYP1A2	CYP1A2	Calculating...	Calculating...
Metabolism	Cytochrome CYP2C19	CYP2C19	Calculating...	Calculating...
Metabolism	Cytochrome CYP2C9	CYP2C9	Calculating...	Calculating...
Metabolism	Cytochrome CYP2D6	CYP2D6	Calculating...	Calculating...

Classification	Target	Shorthand	Prediction	Probability
Metabolism	Cytochrome CYP3A4	CYP3A4	Calculating...	Calculating...
Metabolism	Cytochrome CYP2E1	CYP2E1	Calculating...	Calculating...

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