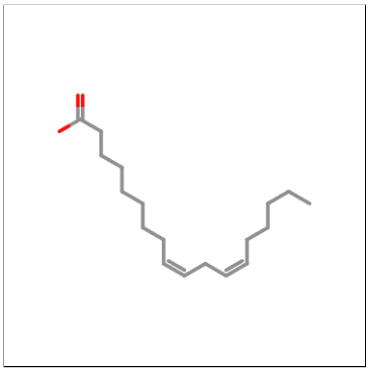
## Oral toxicity prediction results for input compound



**Predicted LD50: 10000mg/kg**

**Predicted Toxicity Class: 6**

| 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|

**Average similarity: 100%**

**Prediction accuracy: 100%**

20% 40% 60% 80%

| Name | CCCCC/C=CC/C=CCCC( |
|---|---|
| Molweight | 280.45 |
| Number of hydrogen bond acceptors | 2 |
| Number of hydrogen bond donors | 1 |
| Number of atoms | 20 |
| Number of bonds | 19 |
| Number of rotable bonds | 14 |
| Molecular refractivity | 89.46 |
| Topological Polar Surface Area | 37.3 |
| octanol/water partition coefficient(logP) | 5.88 |

## Toxicity Model Report

Copy Excel CSV PDF

| Classification | Target | Shorthand | Prediction | Probability |
|---|---|---|---|---|
| Organ toxicity | Hepatotoxicity | dili | Inactive | 0.55 |
| Organ toxicity | Neurotoxicity | neuro | Inactive | 0.91 |
| Organ toxicity | Nephrotoxicity | nephro | Inactive | 0.55 |
| Organ toxicity | Respiratory toxicity | respi | Inactive | 0.84 |
| Organ toxicity | Cardiotoxicity | cardio | Inactive | 0.99 |
| Toxicity end points | Carcinogenicity | carcino | Inactive | 0.64 |
| Toxicity end points | Immunotoxicity | immuno | Inactive | 0.96 |
| Toxicity end points | Mutagenicity | mutagen | Inactive | 1.0 |
| Toxicity end points | Cytotoxicity | cyto | Inactive | 0.71 |
| Toxicity end points | BBB-barrier | bbb | **Active** | 0.89 |
| Toxicity end points | Ecotoxicity | eco | **Active** | 0.65 |
| Toxicity end points | Clinical toxicity | clinical | Inactive | 0.61 |
| Toxicity end points | Nutritional toxicity | nutri | Inactive | 0.89 |
| Tox21-Nuclear receptor signalling pathways | Aryl hydrocarbon Receptor (AhR) | nr_ahr | Inactive | 1.0 |
| Tox21-Nuclear receptor signalling pathways | Androgen Receptor (AR) | nr_ar | Inactive | 1.0 |
| Tox21-Nuclear receptor signalling pathways | Androgen Receptor Ligand Binding Domain (AR-LBD) | nr_ar_lbd | Inactive | 1.0 |
| Tox21-Nuclear receptor signalling pathways | Aromatase | nr_aromatase | Inactive | 1.0 |
| Tox21-Nuclear receptor signalling pathways | Estrogen Receptor Alpha (ER) | nr_er | Inactive | 1.0 |
| Tox21-Nuclear receptor signalling pathways | Estrogen Receptor Ligand Binding Domain (ER-LBD) | nr_er_lbd | Inactive | 1.0 |
| Tox21-Nuclear receptor signalling pathways | Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma) | nr_ppar_gamma | **Active** | 0.90 |
| Tox21-Stress response pathways | Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE) | sr_are | **Active** | 0.91 |
| Tox21-Stress response pathways | Heat shock factor response element (HSE) | sr_hse | **Active** | 0.91 |
| Tox21-Stress response pathways | Mitochondrial Membrane Potential (MMP) | sr_mmp | Inactive | 1.0 |
| Tox21-Stress response pathways | Phosphoprotein (Tumor Supressor) p53 | sr_p53 | Inactive | 1.0 |
| Tox21-Stress response pathways | ATPase family AAA domain-containing protein 5 (ATAD5) | sr_atad5 | Inactive | 1.0 |
| Molecular Initiating Events | Thyroid hormone receptor alpha (THRα) | mie_thr_alpha | Inactive | 0.90 |
| Molecular Initiating Events | Thyroid hormone receptor beta (THRβ) | mie_thr_beta | Inactive | 0.78 |
| Molecular Initiating Events | Transtyretrin (TTR) | mie_ttr | Inactive | 0.97 |
| Molecular Initiating Events | Ryanodine receptor (RYR) | mie_ryr | Inactive | 0.98 |
| Molecular Initiating Events | GABA receptor (GABAR) | mie_gabar | Inactive | 0.96 |
| Molecular Initiating Events | Glutamate N-methyl-D-aspartate receptor (NMDAR) | mie_nmdar | Inactive | 0.92 |
| Molecular Initiating Events | alpha-amino-3-hydroxy-5-methyl-4-isoxazolepropionate receptor (AMPAR) | mie_ampar | Inactive | 0.97 |
| Molecular Initiating Events | Kainate receptor (KAR) | mie_kar | Inactive | 0.99 |
| Molecular Initiating Events | Achetylcholinesterase (AChE) | mie_ache | Inactive | 0.55 |
| Molecular Initiating Events | Constitutive androstane receptor (CAR) | mie_car | Inactive | 0.98 |
| Molecular Initiating Events | Pregnane X receptor (PXR) | mie_pxr | Inactive | 0.92 |
| Molecular Initiating Events | NADH-quinone oxidoreductase (NADHOX) | mie_nadhox | Inactive | 0.97 |
| Molecular Initiating Events | Voltage gated sodium channel (VGSC) | mie_vgsc | Inactive | 0.95 |

| Classification | Target | Shorthand | Prediction | Probability |
|---|---|---|---|---|
| Molecular Initiating Events | Na+/I- symporter (NIS) | mie_nis | Inactive | 0.98 |
| Metabolism | Cytochrome CYP1A2 | CYP1A2 | Inactive | 0.91 |
| Metabolism | Cytochrome CYP2C19 | CYP2C19 | Inactive | 0.98 |
| Metabolism | Cytochrome CYP2C9 | CYP2C9 | Inactive | 0.69 |
| Metabolism | Cytochrome CYP2D6 | CYP2D6 | Inactive | 0.88 |
| Metabolism | Cytochrome CYP3A4 | CYP3A4 | Inactive | 1.0 |
| Metabolism | Cytochrome CYP2E1 | CYP2E1 | Inactive | 0.99 |

## 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 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | | | | | |