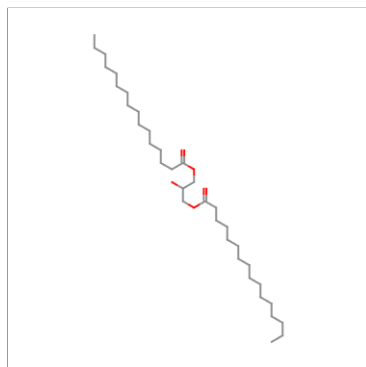
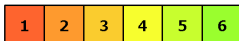


Oral toxicity prediction results for input compound



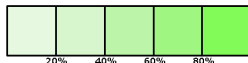
Predicted LD50: 5000mg/kg

Predicted Toxicity Class: 5



Average similarity: 97.56%

Prediction accuracy: 72.9%



| | |
|---|------------------|
| Name | CCCCCCCCCCCCCCCC |
| Molweight | 568.91 |
| Number of hydrogen bond acceptors | 5 |
| Number of hydrogen bond donors | 1 |
| Number of atoms | 40 |
| Number of bonds | 39 |
| Number of rotatable bonds | 34 |
| Molecular refractivity | 174.09 |
| Topological Polar Surface Area | 72.83 |
| octanol/water partition coefficient(logP) | 10.4 |

Toxicity Model Report

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| Classification | Target | Shorthand | Prediction | Probability |
|--|---|---------------|------------|-------------|
| Organ toxicity | Hepatotoxicity | dili | Inactive | 0.89 |
| Organ toxicity | Neurotoxicity | neuro | Inactive | 0.94 |
| Organ toxicity | Nephrotoxicity | nephro | Active | 0.56 |
| Organ toxicity | Respiratory toxicity | respi | Inactive | 0.82 |
| Organ toxicity | Cardiotoxicity | cardio | Inactive | 0.96 |
| Toxicity end points | Carcinogenicity | carcino | Active | 0.56 |
| Toxicity end points | Immunotoxicity | immuno | Inactive | 0.98 |
| Toxicity end points | Mutagenicity | mutagen | Inactive | 0.61 |
| Toxicity end points | Cytotoxicity | cyto | Inactive | 0.85 |
| Toxicity end points | BBB-barrier | bbb | Active | 0.81 |
| Toxicity end points | Ecotoxicity | eco | Inactive | 0.68 |
| Toxicity end points | Clinical toxicity | clinical | Inactive | 0.64 |
| Toxicity end points | Nutritional toxicity | nutri | Inactive | 0.94 |
| 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 | 0.99 |
| Tox21-Nuclear receptor signalling pathways | Estrogen Receptor Alpha (ER) | nr_er | Inactive | 0.89 |
| Tox21-Nuclear receptor signalling pathways | Estrogen Receptor Ligand Binding Domain (ER-LBD) | nr_er_lbd | Inactive | 0.99 |
| Tox21-Nuclear receptor signalling pathways | Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma) | nr_ppar_gamma | Inactive | 0.95 |
| Tox21-Stress response pathways | Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE) | sr_are | Inactive | 0.96 |
| Tox21-Stress response pathways | Heat shock factor response element (HSE) | sr_hse | Inactive | 0.96 |
| Tox21-Stress response pathways | Mitochondrial Membrane Potential (MMP) | sr_mmp | Inactive | 1.0 |
| Tox21-Stress response pathways | Phosphoprotein (Tumor Suppressor) p53 | sr_p53 | Inactive | 0.98 |
| Tox21-Stress response pathways | ATPase family AAA domain-containing protein 5 (ATAD5) | sr_atad5 | Inactive | 0.99 |
| 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 | Transthyretin (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 (AMPA) | mie_ampar | Inactive | 0.97 |
| Molecular Initiating Events | Kainate receptor (KAR) | mie_kar | Inactive | 0.99 |
| Molecular Initiating Events | Achetylcholinesterase (AChE) | mie_ache | Inactive | 0.89 |
| 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 |

