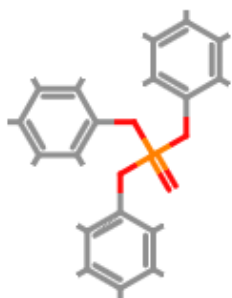
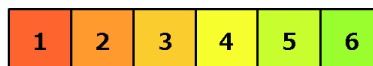


Oral toxicity prediction results for input compound



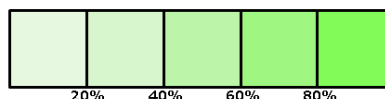
Predicted LD50: 1320mg/kg

Predicted Toxicity Class: 4



Average similarity: 100%

Prediction accuracy: 100%



Name	Triphenyl phosphite
Molweight	326.28
Number of hydrogen bond acceptors	4
Number of hydrogen bond donors	0
Number of atoms	23
Number of bonds	25
Number of rotatable bonds	6
Molecular refractivity	88.82
Topological Polar Surface Area	54.57
octanol/water partition coefficient(logP)	5.33

Toxicity Model Report

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Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.74
Organ toxicity	Neurotoxicity	neuro	Inactive	0.85
Organ toxicity	Nephrotoxicity	nephro	Inactive	0.56
Organ toxicity	Respiratory toxicity	respi	Inactive	0.98
Organ toxicity	Cardiotoxicity	cardio	Inactive	0.69
Toxicity end points	Carcinogenicity	carcino	Inactive	0.76
Toxicity end points	Immunotoxicity	immuno	Inactive	0.99

Classification	Target	Shorthand	Prediction	Probability
Toxicity end points	<u>Mutagenicity</u>	mutagen	Inactive	0.96
Toxicity end points	<u>Cytotoxicity</u>	cyto	Inactive	0.83
Toxicity end points	<u>BBB-barrier</u>	bbb	Active	0.82
Toxicity end points	<u>Ecotoxicity</u>	eco	Active	0.73
Toxicity end points	<u>Clinical toxicity</u>	clinical	Inactive	0.71
Toxicity end points	<u>Nutritional toxicity</u>	nutri	Inactive	0.54
Tox21-Nuclear receptor signalling pathways	<u>Aryl hydrocarbon Receptor (AhR)</u>	nr_ahr	Active	0.61
Tox21-Nuclear receptor signalling pathways	<u>Androgen Receptor (AR)</u>	nr_ar	Inactive	0.99
Tox21-Nuclear receptor signalling pathways	<u>Androgen Receptor Ligand Binding Domain (AR-LBD)</u>	nr_ar_lbd	Inactive	1.0
Tox21-Nuclear receptor signalling pathways	<u>Aromatase</u>	nr_aromatase	Inactive	0.99
Tox21-Nuclear receptor signalling pathways	<u>Estrogen Receptor Alpha (ER)</u>	nr_er	Active	0.99
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	0.99
Tox21-Stress response pathways	<u>Heat shock factor response element (HSE)</u>	sr_hse	Inactive	0.99
Tox21-Stress response pathways	<u>Mitochondrial Membrane Potential (MMP)</u>	sr_mmp	Active	0.99
Tox21-Stress response pathways	<u>Phosphoprotein (Tumor Suppressor)_p53</u>	sr_p53	Inactive	0.99
Tox21-Stress response pathways	<u>ATPase family AAA domain-containing protein 5 (ATAD5)</u>	sr_atad5	Inactive	0.99
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 (RYP)</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

