|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| SUBSTÂNCIA | Caffeico | Kaempferol 3–rutinosídeo | Rutina | Lupeol | pseudotaraxasterol | 3-O-β-D-glucopiranosilβ-sitosterol- 3-O-beta-d-glucopyranosylsitosterol | 3-O-β-D-glucopiranosil-estigmasterol - Stigmasterol glucoside |
| Código Pubchem | 689043 | [5318767](https://pubchem.ncbi.nlm.nih.gov/compound/5318767) | [5280805](https://pubchem.ncbi.nlm.nih.gov/compound/5280805) | [259846](https://pubchem.ncbi.nlm.nih.gov/compound/259846) | [604983](https://pubchem.ncbi.nlm.nih.gov/compound/604983) | [12309067](https://pubchem.ncbi.nlm.nih.gov/compound/12309067) | [6602508](https://pubchem.ncbi.nlm.nih.gov/compound/6602508) |
| [Hepatotoxicity](https://comptox.charite.de/protox3/index.php?site=models#organ/model_liver) | Inactive | Inactive | Active | Inactive | Inactive | Inactive | Inactive |
| [Neurotoxicity](https://comptox.charite.de/protox3/index.php?site=models#organ/model_neuro) | Inactive | Inactive | Active | Active | Active | Inactive | Inactive |
| [Nephrotoxicity](https://comptox.charite.de/protox3/index.php?site=models#organ/model_nephro) | Active | Active | Inactive | Inactive | Inactive | Inactive | Active |
| [Respiratory toxicity](https://comptox.charite.de/protox3/index.php?site=models#organ/model_respi) | Inactive | Active | Active | Active | Active | Active | Inactive |
| [Cardiotoxicity](https://comptox.charite.de/protox3/index.php?site=models#organ/model_cardio) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Active |
| [Carcinogenicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_carcinogenecity) | Active | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Immunotoxicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_immunotoxicity) | Inactive | Active | Active | Active | Active | Inactive | Active |
| [Mutagenicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_mutagenecity) | Inactive | Inactive | Inactive | Inactive | Inactive | Active | Inactive |
| [Cytotoxicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_cytotoxicity) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [BBB-barrier](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_bbb) | Active | Inactive | Inactive | Active | Active | Inactive | Inactive |
| [Ecotoxicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_eco) | Inactive | Inactive | Active | Active | Active | Inactive | Inactive |
| [Clinical toxicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_clinical) | Active | Active | Inactive | Active | Active | Inactive | Inactive |
| [Nutritional toxicity](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_endpoints/model_nutri) | Inactive | Active | Inactive | Active | Active | Active | Active |
| [Aryl hydrocarbon Receptor (AhR)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_AhR) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Androgen Receptor (AR)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_AR) | Active | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Androgen Receptor Ligand Binding Domain (AR-LBD)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_AR_LBD) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Aromatase](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_AROMATASE) | Inactive | Inactive | Active | Inactive | Inactive | Inactive | Inactive |
| [Estrogen Receptor Alpha (ER)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_ER) | Inactive | Inactive | Active | Inactive | Inactive | Inactive | Inactive |
| [Estrogen Receptor Ligand Binding Domain (ER-LBD)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_ER_LBD) | Inactive | Inactive | Active | Inactive | Inactive | Inactive | Inactive |
| [Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/nuclear_receptor_signalling_patways/MODEL_ppar_gamma) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/Stress_response_pathways/MODEL_ARE) | Inactive | Inactive | Inactive | Active | Inactive | Inactive | Inactive |
| [Heat shock factor response element (HSE)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/Stress_response_pathways/MODEL_HSE) | Inactive | Inactive | Inactive | Active | Inactive | Inactive | Inactive |
| [Mitochondrial Membrane Potential (MMP)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/Stress_response_pathways/MODEL_MMP) | Inactive | Inactive | Inactive | Inactive | Active | Inactive | Inactive |
| [Phosphoprotein (Tumor Supressor) p53](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/Stress_response_pathways/MODEL_P53) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| [ATPase family AAA domain-containing protein 5 (ATAD5)](https://comptox.charite.de/protox3/index.php?site=models#Toxicological_pathways/TOX_21/Stress_response_pathways/MODEL_STAD5) | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive | Inactive |
| Massa molar | 180.16 | 594.52 | 371.52 | 412.69 | 426.72 | 576.85 | 560.81 |
| Número de aceitadores de ligações de hidrogênio | 4 | 14 | 2 | 1 | 1 | 6 | 6 |
| Número de doadores de ligações de hidrogênio | 3 | 9 | 0 | 1 | 1 | 4 | 4 |
| Área de superfície polar topológica | 77.76 | 249.2 | 12.47 | 20.23 | 20.23 | 99.38 | 99.38 |
| Coeficiente de partição octanol/água (logP) | 1.2 | -1.39 | 6 | 7.63 | 8.02 | 5.85 | 5.23 |