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| --- | --- |
| **Identifier** | Compound identifier/ trivial name |
| **Structure** | 2D |
| **SMILES** | SMILES representation |
| **Mode of action** | MOA |
| **Superclass** | according to program Classyfire |
| **Class** | according to program Classyfire |
| **\*Risks\*** | ADMET\_Risk [0.000,8.703] green, Absn\_Risk [0.000,6.578] blue, MUT\_Risk [0.000,1.800] pink, TOX\_Risk [0.000,2.412] yellow |
| **\*PCB\*** | Physicochemical and Biopharmaceutical properties: MWt [163.242,792.027] green, N\_FrRotB [0.000,12.000] blue, S+logP [-6.287,7.667] pink, S+Peff [0.048,11.943]  yellow, log(S+Sw) [-3.584,2.507] red |
| **ECCS\_Class** | ECCS class describing major clearance mechanism. Based on Varma et al. publication. 1A=metabolism, 1B=hepatic uptake, 2=metabolism, 3A=renal,  3B=hepatic uptake or renal, 4=renal. |
| **RuleOf5\_Code** | Lipinski's Rule of 5 codes: LP=log P, Hb=number of hydrogen bond donor hydrogens, MW=molecular weight, NO=number of N and O atoms. |
| **ADMET\_Code** | Full ADMET Risk rule codes: Size, RotB=rotatable bonds, HBD=H-bond donors, HBA=H-bond acceptors, ch=charge, Kow=lipophilicity, Peff=permeability,  Sw=water solubility, fu=fraction unbound, Vd=volume of distribution, hERG=hERG inhibition, rat=acute rat toxicity, Xr=carcinogenicity in rat,  Xm=carcinogenicity in mice, HEPX=hepatotoxicity, MUT=likely Ames positive; 1A2=high clearance by CYP 1A2, etc., CL=high microsomal clearance.  WARNING: rules related to unlicensed modules are turned off, which may result in missing codes. |
| **S+logP** | Simulations Plus model of log P. RMSE/MAE = 0.30/0.23. |
| **S+Peff** | Effective human jejunal permeability (cm/s x 10^4). RMSE/MAE = 0.31/0.25 log units. |
| **S+Sw** | Water solubility (mg/mL). RMSE/MAE = 0.59/0.45 (2D) and 0.57/0.43 (3D) in log units. |
| **S+MDCK** | Apparent MDCK Transwell permeability (cm/s x 10^7). RMSE/MAE = 0.47/0.48 (2D and 3D) log units. |
| **Perm\_Cornea** | Permeability through the rabbit cornea (cm/s x 10^7). RMSE/MAE = 0.40/0.32 log units. |
| **Perm\_Skin** | Permeability through human skin (cm/s x 10^7). RMSE/MAE = 0.48/0.38 log units. |
| **hum\_fup%** | Percent UNBOUND to blood plasma proteins in human. RMSE/MAE = 0.43/0.32 (2D) log units. |
| **RBP** | Blood to plasma concentration ratio in human. RMSE/MAE = 0.09/0.07 (2D) log units. |
| **S+fumic** | Fraction unbound in human liver microsomes at 1 mg/mL microsomal protein concentration. RMSE/MAE = 0.18/0.13. |
| **MW** | Relative molecularmass/Molecula Weighzt |
| **HBA** | Number of H-Bond Acceptors |
| **HBD** | Number of H-Bond Donors |
| **TPSA\_DW** | Topological Polar Surface Area calculated by DataWarrior (other parameters are calculated by ADMET Predictor) |
| **RB\_DW** | Number of Rotatable Bonds calculated by DataWarrior (other parameters are calculated by ADMET Predictor) |
| **BBB\_Filter** | Predicts whether or not a compound can penetrate the Blood Brain Barrier. Overall accuracy = 92%. |
| **LogBB** | Logarithm of the Brain/Blood partition coefficient. RMSE/MAE = 0.37/0.28 (2D and 3D). |