|  |  |  |
| --- | --- | --- |
| Physicochemical Properties  | Compound K | Standard Range |
| Molecular weight (g/mol) | 622.9 |  < 500 |
| Num. rotatable bonds | 7 |   |
| Num. H-bond acceptors | 8 |  ≤ 10 |
| Hydrogen bond donor | 6 |  ≤ 5 |
| Molar Refractivity | 172.26 | 40–130 |
| TPSA (Å2) | 139.84 |  < 140 Å2 |
| Lipinski | Yes; 2 violation |   |
| Bioavailability Score | 0.17 | ˃0.1 |
| *ADME*  |
| Human Intestinal Absorption | 54.344 |   |
| GI absorption | Low |   |
| Blood-brain Barrier Permeability | -1.038 | 0–1 |
| Volume distribution | 1.061 | 0.04-20L/Kg |
| Plasma-protein binding | 93.57% | <90% |
| Total Clearance (log ml/min/kg) | 0.46 |   |
| CYP1A2 inhibitor  | No | 0–1 |
| CYP2C19 inhibitor  | No | 0–1 |
| CYP2C9 inhibitor  | No | 0–1 |
| CYP2D6 inhibitor  | No | 0–1 |
| CYP3A4 inhibitor  | No | 0–1 |
| *Toxicity*  |
| Hepatotoxicity | Active (0.69) | 0–1 |
| Carcinogenesis | Inactive (0.62) | 0–1 |
| Immunotoxicity | Active (0.96) | 0–1 |
| Mutagenicity | Inactive (0.97) | 0–1 |
| Cytotoxicity | Inactive (0.93) | 0–1 |
| Mitochondrial Membrane Potential | Inactive (0.70) | 0–1 |