|  |  |  |
| --- | --- | --- |
| 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 |