|  |  |  |
| --- | --- | --- |
|  | Compound (1) | Compound (2) |
| [miLogP](https://www.molinspiration.com/services/logp.html) | 1.81 | 3.37 |
| [TPSA](https://www.molinspiration.com/services/psa.html) | 69.88 | 83.11 |
| natoms | 15 | 20 |
| MW | 226,67 | 290.71 |
| nON | 5 | 6 |
| nOHNH | 2 | 1 |
| nviolations | 0 | 0 |
| nrotb | 3 | 4 |
| GPCR ligand | -0.78 | -0.70 |
| Ion channel modulator | -0.62 | -0.70 |
| Kinase inhibitor | -0.74 | -0.55 |
| Nuclear receptor ligand | -1.32 | -0.94 |
| Protease inhibitor | -1.32 | -1.02 |
| Enzyme inhibitor | -0.43 | -0.49 |