|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **MW** | | **LogP** | | **nHA** | | **nHD** | |
| **active** | **inactive** | **active** | **inactive** | **active** | **inactive** | **active** | **inactive** |
| ***p*-value** | 4.01332667e-11 | | 0.15113827 | | 1.37885476e-09 | | 0.00019855 | |
| **min** | 217.29 | 162.21 | -5.67 | -7.10 | 4 | 1 | 1 | 0 |
| **Q1** | 368.24 | 259.58 | -0.86 | -1.09 | 7 | 4 | 2 | 2 |
| **median** | 413.46 | 322.45 | -0.13 | 0.65 | 7 | 6 | 3 | 2 |
| **mean** | 422.54 | 348.45 | 0.38 | 0.67 | 7.53 | 6.14 | 2.83 | 2.37 |
| **std** | 79.47 | 124.63 | 1.96 | 2.47 | 2.05 | 2.57 | 1.15 | 1.28 |
| **Q3** | 468.91 | 429.56 | 1.59 | 2.72 | 9 | 7 | 3 | 3 |
| **max** | 703.80 | 1174.44 | 5.35 | 5.32 | 16 | 25 | 8 | 8 |
| **skew** | 0.34 | 2.30 | 0.24 | -0.36 | 0.72 | 2.81 | 1.04 | 0.92 |
| **kurtosis** | 0.99 | 12.23 | 0.15 | -0.24 | 2.20 | 17.79 | 3.17 | 2.02 |
|  | **TPSA** | | **nRot** | | **nHET** | | **Aro** | |
| **active** | **inactive** | **active** | **inactive** | **active** | **inactive** | **active** | **inactive** |
| ***p*-value** | 7.03534658e-09 | | 8.51495926e-05 | | 1.04832227e-12 | | 0.02483612 | |
| **min** | 26.36 | 38.77 | 2 | 0 | 5 | 2 | 0 | 0 |
| **Q1** | 106.94 | 97.33 | 7 | 5 | 7 | 5 | 1 | 0 |
| **median** | 127.25 | 108.21 | 8 | 7 | 8 | 6 | 1 | 1 |
| **mean** | 130.39 | 115.80 | 8.92 | 7.34 | 8.26 | 6.87 | 1.36 | 1.14 |
| **std** | 26.36 | 33.93 | 3.46 | 4.07 | 1.86 | 2.47 | 0.79 | 0.90 |
| **Q3** | 137.02 | 126.82 | 11 | 10 | 9 | 8 | 2 | 2 |
| **max** | 239.98 | 351.81 | 17 | 36 | 16 | 25 | 4 | 4 |
| **skew** | 1.62 | 2.95 | 0.30 | 2.38 | 1.29 | 3.13 | 0.66 | 0.38 |
| **kurtosis** | 3.88 | 17.33 | -0.47 | 14.92 | 3.01 | 19.02 | 1.29 | -0.37 |