|  |  |  |
| --- | --- | --- |
|  | MBDTA-1  | MBDTA-2 |
| Molecular mass (Da) | 293.3 | 293.3 |
| clog*P* | 1.96 | 1.96 |
| clog*S* | -2.375 | -2.379 |
| pKa | 3.115 | 3.143 |
| tPSA | 83.91 | 83.91 |
| #H-bond donors | 1 | 1 |
| #H-bond acceptors  | 6 | 6 |