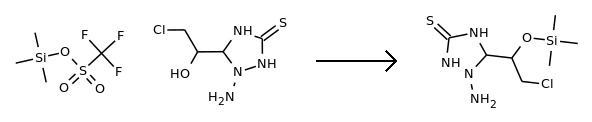
[ASKCOS](https://askcos.mit.edu/)



Solvent:

ClCCl

Τέλος φόρμας

| **Rank** | **Product** | **Probability** | **Max. Score** | **Molecular Weight** | **Predict impurities** | **Predict regio-selectivities** |
| --- | --- | --- | --- | --- | --- | --- |
| 1 | C[Si](C)(C)OC(CCl)C1NC(=S)NN1N | 0.8973 | -67.910 | 268.8 |  |  |
| 2 | O=S(=O)(O)C(F)(F)F | 0.0884 | -70.227 | 150.1 |  |  |
| 3 | NN1N=C=NC1C(O)CCl | 0.0035 | -73.443 | 162.6 |  |  |
| 4 | NN1NC=NC1C(O)CCl | 0.0031 | -73.576 | 164.6 |  |  |
| 5 | NN1NC=NC1C(S)CCl | 0.0022 | -73.939 | 180.7 |  |  |
| 6 | NN1NC(=S)NC1C(CCl)OS(=O)(=O)C(F)(F)F | 0.0013 | -74.434 | 328.7 |  |  |
| 7 | NN1NC2=NC1C(CCl)O2 | 0.0008 | -74.924 | 162.6 |  |  |
| 8 | NN1N=C=NC1C(S)CCl | 0.0008 | -74.991 | 178.6 |  |  |
| 9 | O=S(=O)(NN1NC(=S)NC1C(O)CCl)C(F)(F)F | 0.0005 | -75.443 | 328.7 |  |  |
| 10 | NN1NCNC1C(S)CCl | 0.0005 | -75.497 | 182.7 |  |  |
| 11 | NN1N=CNC1C(O)CCl | 0.0003 | -75.822 | 164.6 |  |  |
| 12 | NN1NC(=S)NC1CCCl | 0.0003 | -75.926 | 180.7 |  |  |
| 13 | NN1N=CNC1C(S)CCl | 0.0002 | -76.248 | 180.7 |  |  |
| 14 | NN1NC(O)=NC1CCCl | 0.0002 | -76.321 | 164.6 |  |  |
| 15 | OC(CCl)C1NNC(=S)N1 | 0.0001 | -76.609 | 181.6 |  |  |
| 16 | OC(CCl)C1N=C2NN1N2 | 0.0001 | -76.844 | 162.6 |  |  |
| 17 | NN1NCNC1C(O)CCl | 0.0001 | -76.926 | 166.6 |  |  |
| 18 | NN1N=C2NC1C(CCl)O2 | 0.0001 | -77.532 | 162.6 |  |  |
| 19 | O=[SH](=O)C(F)(F)F | 0.0000 | -77.812 | 134.1 |  |  |
| 20 | NC1=NC(C(O)CCl)NN1 | 0.0000 | -77.907 | 164.6 |  |  |
| 21 | C[Si](C)(C)OC1NC(CCCl)N(N)N1 | 0.0000 | -77.980 | 238.8 |  |  |
| 22 | NN1N=C(O)NC1CCCl | 0.0000 | -78.164 | 164.6 |  |  |
| 23 | SC(CCl)C1N=C2NN1N2 | 0.0000 | -78.620 | 178.6 |  |  |
| 24 | OC(CCl)C1Nc2nn1[nH]2 | 0.0000 | -79.399 | 162.6 |  |  |
| 25 | NN1NC(O)=NC1C(S)CCl | 0.0000 | -79.495 | 196.7 |  |  |
| 26 | NN1NC=NC1C(O)(S)CCl | 0.0000 | -79.597 | 196.7 |  |  |
| 27 | NN1N=C=NC1C(O)(S)CCl | 0.0000 | -79.833 | 194.6 |  |  |
| 28 | C[Si](C)(C)O[SH](=O)(O)C(F)(F)F | 0.0000 | -80.160 | 224.3 |  |  |
| 29 | NN1NC2NC1C(CCl)O2 | 0.0000 | -80.702 | 164.6 |  |  |
| 30 | C[Si](C)(C)OS(=O)C(F)(F)F | 0.0000 | -80.896 | 206.3 |  |  |
| 31 | SC(CCl)C1Nc2nn1[nH]2 | 0.0000 | -81.449 | 178.6 |  |  |
| 32 | O=S(=O)(N1C2=NC(C(O)CCl)N1N2)C(F)(F)F | 0.0000 | -81.582 | 294.6 |  |  |
| 33 | NN1NCNC1C(O)(S)CCl | 0.0000 | -81.733 | 198.7 |  |  |
| 34 | C[Si](C)(C)OC(CCl)C1NC(=S)NN1NS(=O)(=O)C(F)(F)F | 0.0000 | -81.785 | 400.9 |  |  |
| 35 | NC1=NNC(C(O)CCl)N1 | 0.0000 | -82.147 | 164.6 |  |  |
| 36 | NN1N=C(O)NC1C(S)CCl | 0.0000 | -82.303 | 196.7 |  |  |
| 37 | NN1NC(=S)NC1C(CCl)OS(=O)C(F)(F)F | 0.0000 | -82.523 | 312.7 |  |  |
| 38 | C[Si](C)(C)OC(Cl)CC1NC(=S)NN1N | 0.0000 | -82.530 | 268.8 |  |  |
| 39 | NN1N=CNC1C(O)(S)CCl | 0.0000 | -82.548 | 196.7 |  |  |
| 40 | CC1NC(=S)NN1N | 0.0000 | -82.772 | 132.2 |  |  |
| 41 | NN1NC=NC1CS | 0.0000 | -82.822 | 132.2 |  |  |
| 42 | NN1NC2=NC1C(S)(CCl)O2 | 0.0000 | -82.869 | 194.6 |  |  |
| 43 | NN1NC(=S)NC1CO | 0.0000 | -82.881 | 148.2 |  |  |
| 44 | CC1N=C(O)NN1N | 0.0000 | -83.301 | 116.1 |  |  |
| 45 | C[Si](C)(C)O[SH](=O)(OC(CCl)C1NC(=S)NN1N)C(F)(F)F | 0.0000 | -83.327 | 402.9 |  |  |
| 46 | C[Si](C)(C)O[SH](=O)(NN1NC(=S)NC1C(O)CCl)C(F)(F)F | 0.0000 | -83.370 | 402.9 |  |  |
| 47 | OC(S)(CCl)C1N=C2NN1N2 | 0.0000 | -83.442 | 194.6 |  |  |
| 48 | NC1=NC(C(O)(S)CCl)NN1 | 0.0000 | -83.678 | 196.7 |  |  |
| 49 | O=S(NN1NC(=S)NC1C(O)CCl)C(F)(F)F | 0.0000 | -84.460 | 312.7 |  |  |
| 50 | O=[SH]C(F)(F)F | 0.0000 | -84.723 | 118.1 |  |  |
| 51 | O=S(=O)(NN1NC(=S)NC1CCCl)C(F)(F)F | 0.0000 | -84.932 | 312.7 |  |  |
| 52 | O=S(=O)(n1c2nn1C(C(O)CCl)N2)C(F)(F)F | 0.0000 | -84.935 | 294.6 |  |  |
| 53 | NN1NC(OS(=O)(=O)C(F)(F)F)NC1CCCl | 0.0000 | -85.053 | 298.7 |  |  |
| 54 | CC1NC(O)=NN1N | 0.0000 | -85.089 | 116.1 |  |  |
| 55 | NN1N=CNC1CS | 0.0000 | -85.120 | 132.2 |  |  |
| 56 | NN1NCNC1CS | 0.0000 | -85.469 | 134.2 |  |  |
| 57 | NN1NC(=S)NC1C1OC1Cl | 0.0000 | -85.676 | 194.6 |  |  |
| 58 | NN1N=C=NC1C(O)S | 0.0000 | -85.692 | 146.2 |  |  |
| 59 | NN1N=C2NC1C(S)(CCl)O2 | 0.0000 | -85.721 | 194.6 |  |  |
| 60 | C[Si](C)(C)OC(CCl)C1NNC(=S)N1 | 0.0000 | -85.848 | 253.8 |  |  |
| 61 | NN1NC2=NC1C(S)O2 | 0.0000 | -86.126 | 146.2 |  |  |
| 62 | OC(S)(CCl)C1Nc2nn1[nH]2 | 0.0000 | -86.160 | 194.6 |  |  |
| 63 | C[Si](C)(C)O[SH](N)(=O)C(F)(F)F | 0.0000 | -86.519 | 223.3 |  |  |
| 64 | NN1NC(=S)NC1CC(O)Cl | 0.0000 | -87.649 | 196.7 |  |  |
| 65 | O=[SH]1(C(F)(F)F)NN2NC(=S)NC2C(CCl)O1 | 0.0000 | -87.917 | 312.7 |  |  |
| 66 | NC1=NNC(C(O)(S)CCl)N1 | 0.0000 | -88.034 | 196.7 |  |  |
| 67 | OC(S)C1N=C2NN1N2 | 0.0000 | -88.154 | 146.2 |  |  |
| 68 | NN1NC=NC1C(O)S | 0.0000 | -88.255 | 148.2 |  |  |
| 69 | C[Si](C)(C)O[SH](=O)(N1C2=NC(C(O)CCl)N1N2)C(F)(F)F | 0.0000 | -88.300 | 368.8 |  |  |
| 70 | NN1NC2NC1C(S)(CCl)O2 | 0.0000 | -88.585 | 196.7 |  |  |
| 71 | NN1N=C2NC1C(S)O2 | 0.0000 | -88.815 | 146.2 |  |  |
| 72 | NN1NC=NC1C(S)C(O)Cl | 0.0000 | -89.337 | 196.7 |  |  |
| 73 | NN1NC2=NC1CC(Cl)O2 | 0.0000 | -89.523 | 162.6 |  |  |
| 74 | NN1NC(=S)NC1COCCl | 0.0000 | -89.612 | 196.7 |  |  |
| 75 | C[Si](C)(C)OC(CCl)C1NC(=S)NN1NS(=O)C(F)(F)F | 0.0000 | -89.699 | 384.9 |  |  |
| 76 | O=[SH](O)(NN1NC(=S)NC1CCCl)C(F)(F)F | 0.0000 | -89.741 | 314.7 |  |  |
| 77 | NN1NC(=S)NC1CC(Cl)OS(=O)(=O)C(F)(F)F | 0.0000 | -89.816 | 328.7 |  |  |
| 78 | NN1NCNC1C(S)C(O)Cl | 0.0000 | -90.255 | 198.7 |  |  |