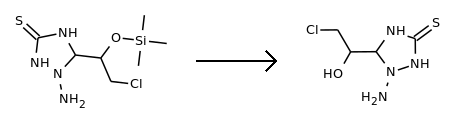
[ASKCOS](https://askcos.mit.edu/)



Reagents:

Cl

Solvent:

CO

Τέλος φόρμας

| **Rank** | **Product** | **Probability** | **Max. Score** | **Molecular Weight** | **Predict impurities** | **Predict regio-selectivities** |
| --- | --- | --- | --- | --- | --- | --- |
| 1 | COCC(O[Si](C)(C)C)C1NC(=S)NN1N | 0.9489 | -65.952 | 264.4 |  |  |
| 2 | C[Si](C)(C)OC(CO)C1NC(=S)NN1N | 0.0146 | -70.124 | 250.4 |  |  |
| 3 | C[Si](C)(C)OC(CCl)C1N=C(Cl)NN1N | 0.0069 | -70.875 | 271.2 |  |  |
| 4 | C[Si](C)(C)OC(CCl)C1N=CNN1N | 0.0053 | -71.133 | 236.8 |  |  |
| 5 | C[Si](C)(C)OC(CCl)C1NCNN1N | 0.0047 | -71.261 | 238.8 |  |  |
| 6 | NN1NC(=S)NC1C(O)CCl | 0.0042 | -71.370 | 196.7 |  |  |
| 7 | O | 0.0037 | -71.495 | 18.0 |  |  |
| 8 | C[Si](C)(C)OC(CCl)C1N=C2NN1N2 | 0.0032 | -71.648 | 234.8 |  |  |
| 9 | C[Si](C)(C)OC(CCl)C1NC=NN1N | 0.0020 | -72.135 | 236.8 |  |  |
| 10 | COC=C(O[Si](C)(C)C)C1NC(=S)NN1N | 0.0015 | -72.390 | 262.4 |  |  |
| 11 | C[Si](C)(C)OC(CCl)C1NC(Cl)=NN1N | 0.0008 | -73.009 | 271.2 |  |  |
| 12 | C[Si](C)(C)OC(CS)C1NCNN1N | 0.0008 | -73.031 | 236.4 |  |  |
| 13 | C[Si](C)(C)OC(CCl)C1NNC(=S)N1 | 0.0007 | -73.154 | 253.8 |  |  |
| 14 | COC(Cl)=C(O[Si](C)(C)C)C1NC(=S)NN1N | 0.0005 | -73.595 | 296.9 |  |  |
| 15 | C[Si](C)(C)OC(CS)C1N=CNN1N | 0.0003 | -74.062 | 234.4 |  |  |
| 16 | C[Si](C)(C)OC(CCl)C1N=C=NN1N | 0.0002 | -74.223 | 234.8 |  |  |
| 17 | CC(O[Si](C)(C)C)C1NC(=S)NN1N | 0.0002 | -74.324 | 234.4 |  |  |
| 18 | C[Si](C)(C)OC(CCl)C(N)N(N)NC(=S)Cl | 0.0002 | -74.494 | 305.3 |  |  |
| 19 | C=C(O[Si](C)(C)C)C1NC(=S)NN1N | 0.0002 | -74.661 | 232.4 |  |  |
| 20 | C[Si](C)(C)OC(CS)C1N=C(Cl)NN1N | 0.0002 | -74.667 | 268.8 |  |  |
| 21 | C[Si](C)(C)OC(CCl)C1N=C(S)NN1N | 0.0001 | -75.008 | 268.8 |  |  |
| 22 | C[Si](C)(C)OC(CCl)C1N=C(N)NN1 | 0.0001 | -75.014 | 236.8 |  |  |
| 23 | COC(Cl)C(O[Si](C)(C)C)C1NC(=S)NN1N | 0.0001 | -75.428 | 298.9 |  |  |
| 24 | C[Si](C)(C)OC(CCl)C1Nc2nn1[nH]2 | 0.0001 | -75.468 | 234.8 |  |  |
| 25 | C[Si](C)(C)OC(CS)C1N=C2NN1N2 | 0.0001 | -75.564 | 232.4 |  |  |
| 26 | CNN(N)C(N)C(CCl)O[Si](C)(C)C | 0.0001 | -75.691 | 240.8 |  |  |
| 27 | C[Si](C)(C)OC(CCl)C(N)N(N)NCCl | 0.0000 | -75.871 | 275.3 |  |  |
| 28 | C[Si](C)(C)OC1CSC2=NC1N(N)N2 | 0.0000 | -76.101 | 232.4 |  |  |
| 29 | C[Si](C)(C)OCC1NC(=S)NN1N | 0.0000 | -76.307 | 220.4 |  |  |
| 30 | C[Si](C)(C)OC(CS)C1NC=NN1N | 0.0000 | -76.424 | 234.4 |  |  |
| 31 | C[Si](C)(C)OC(CCl)C1NC(S)=NN1N | 0.0000 | -76.534 | 268.8 |  |  |
| 32 | C[Si](C)(C)OC(=CCl)C1NC(=S)NN1N | 0.0000 | -76.614 | 266.8 |  |  |
| 33 | C[Si](C)(C)OC(=C(O)Cl)C1NC(=S)NN1N | 0.0000 | -76.681 | 282.8 |  |  |
| 34 | COC(S)=C(O[Si](C)(C)C)C1NCNN1N | 0.0000 | -76.832 | 264.4 |  |  |
| 35 | C[Si](C)(C)OC(CCl)C(N)n1[nH]c(=S)[nH]1 | 0.0000 | -76.940 | 268.8 |  |  |
| 36 | C[Si](C)(C)OC(=CS)C1NCNN1N | 0.0000 | -77.031 | 234.4 |  |  |
| 37 | C[Si](C)(C)OC(CCl)C(N)N(N)NC=S | 0.0000 | -77.041 | 270.9 |  |  |
| 38 | C[Si](C)(C)OC(=CO)C1NC(=S)NN1N | 0.0000 | -77.058 | 248.4 |  |  |
| 39 | C[Si](C)(C)OC(CCl)C(N)N(N)N=C=S | 0.0000 | -77.076 | 268.8 |  |  |
| 40 | C[Si](C)(C)OC(CS)C1NC(Cl)=NN1N | 0.0000 | -77.189 | 268.8 |  |  |
| 41 | C[Si](C)(C)OC(C(O)Cl)C1NC(=S)NN1N | 0.0000 | -77.539 | 284.8 |  |  |
| 42 | C[Si](C)(C)OC(CCl)C(N)N1NCN1 | 0.0000 | -77.668 | 238.8 |  |  |
| 43 | C[Si](C)(C)OC(CS)C1N=C=NN1N | 0.0000 | -77.873 | 232.4 |  |  |
| 44 | C[Si](C)(C)OC(CCl)C1NN=C(N)N1 | 0.0000 | -77.904 | 236.8 |  |  |
| 45 | C[Si](C)(C)OC(CCl)C(N)N(N)N=CCl | 0.0000 | -77.974 | 273.2 |  |  |
| 46 | COC(S)C(O[Si](C)(C)C)C1NCNN1N | 0.0000 | -78.158 | 266.4 |  |  |
| 47 | C[Si](C)(C)OC(=CS)C1N=CNN1N | 0.0000 | -78.211 | 232.4 |  |  |
| 48 | C[Si](C)(C)OC1CSC2=NN(N)C1N2 | 0.0000 | -78.253 | 232.4 |  |  |
| 49 | C[Si](C)(C)OC(=C(Cl)Cl)C1NC(=S)NN1N | 0.0000 | -79.015 | 301.3 |  |  |
| 50 | C=NN(N)C(N)C(CCl)O[Si](C)(C)C | 0.0000 | -79.078 | 238.8 |  |  |
| 51 | COC(S)C(O[Si](C)(C)C)C1N=CNN1N | 0.0000 | -79.083 | 264.4 |  |  |
| 52 | CNN(N)C(N)C(CS)O[Si](C)(C)C | 0.0000 | -79.093 | 238.4 |  |  |
| 53 | C[Si](C)(C)OC(CCl)C(N)n1nc[nH]1 | 0.0000 | -79.735 | 236.8 |  |  |
| 54 | C[Si](C)(C)OC(CS)C1Nc2nn1[nH]2 | 0.0000 | -79.831 | 232.4 |  |  |
| 55 | C[Si](C)(C)OC(=C(S)Cl)C1NCNN1N | 0.0000 | -79.840 | 268.8 |  |  |
| 56 | C[Si](C)(C)OC(=CS)C1NC=NN1N | 0.0000 | -80.411 | 232.4 |  |  |
| 57 | C[Si](C)(C)OC(CS)C(N)N(N)NCCl | 0.0000 | -80.419 | 272.9 |  |  |
| 58 | C[Si](C)(C)OC(CCl)C(N)NNC(N)=S | 0.0000 | -80.475 | 270.9 |  |  |
| 59 | C[Si](C)(C)OC(C(O)S)C1NCNN1N | 0.0000 | -80.579 | 252.4 |  |  |
| 60 | C[Si](C)(C)OC1=CSC2=NC1N(N)N2 | 0.0000 | -80.812 | 230.4 |  |  |
| 61 | C[Si](C)(C)OC1=CSC2=NN(N)C1N2 | 0.0000 | -80.995 | 230.4 |  |  |
| 62 | C[Si](C)(C)OC(C(Cl)Cl)C1NC(=S)NN1N | 0.0000 | -81.020 | 303.3 |  |  |
| 63 | COC1SC2=NC(C1O[Si](C)(C)C)N(N)N2 | 0.0000 | -81.115 | 262.4 |  |  |
| 64 | C[Si](C)(C)OC(CCl)C(N)N(N)NCS | 0.0000 | -81.205 | 272.9 |  |  |
| 65 | C[Si](C)(C)OC1CSCNN(N)C1N | 0.0000 | -81.628 | 236.4 |  |  |
| 66 | C[Si](C)(C)OC(C(S)Cl)C1NCNN1N | 0.0000 | -81.935 | 270.9 |  |  |
| 67 | COC(S)C(O[Si](C)(C)C)C1NC=NN1N | 0.0000 | -81.948 | 264.4 |  |  |
| 68 | C[Si](C)(C)OC(CCl)C(N)N(N)N=CS | 0.0000 | -82.173 | 270.9 |  |  |
| 69 | C[Si](C)(C)OC(CS)C(N)N1NCN1 | 0.0000 | -82.230 | 236.4 |  |  |
| 70 | C[Si](C)(C)OC(CCl)C(N)NNCN | 0.0000 | -82.322 | 240.8 |  |  |
| 71 | C[Si](C)(C)OC(C(S)Cl)C1N=CNN1N | 0.0000 | -82.389 | 268.8 |  |  |
| 72 | C[Si](C)(C)OC(=C(S)Cl)C1N=CNN1N | 0.0000 | -82.836 | 266.8 |  |  |
| 73 | CNN(N)C(N)C(=CS)O[Si](C)(C)C | 0.0000 | -83.051 | 236.4 |  |  |
| 74 | C=NN(N)C(N)C(CS)O[Si](C)(C)C | 0.0000 | -83.150 | 236.4 |  |  |
| 75 | C[Si](C)(C)OC(CCl)C(N)n1nc(Cl)[nH]1 | 0.0000 | -83.541 | 271.2 |  |  |
| 76 | C[Si](C)(C)OC(CCl)C(N)NN=CN | 0.0000 | -83.602 | 238.8 |  |  |
| 77 | CSC1=NC(CO[Si](C)(C)C)N(N)N1 | 0.0000 | -83.740 | 234.4 |  |  |
| 78 | C[Si](C)(C)OC1CSC=NN(N)C1N | 0.0000 | -83.831 | 234.4 |  |  |
| 79 | COC1SC2=NN(N)C(N2)C1O[Si](C)(C)C | 0.0000 | -84.225 | 262.4 |  |  |
| 80 | C[Si](C)(C)OCC1NCNN1N | 0.0000 | -84.237 | 190.3 |  |  |
| 81 | C[Si](C)(C)OC(=C(S)Cl)C1N=C(Cl)NN1N | 0.0000 | -84.357 | 301.3 |  |  |
| 82 | CNN(N)C(N)C(O[Si](C)(C)C)C(S)OC | 0.0000 | -84.512 | 268.5 |  |  |
| 83 | CSC1=NN(N)C(CO[Si](C)(C)C)N1 | 0.0000 | -84.602 | 234.4 |  |  |
| 84 | C[Si](C)(C)OC1C(Cl)SC2=NC1N(N)N2 | 0.0000 | -84.631 | 266.8 |  |  |
| 85 | C[Si](C)(C)OCC1N=CNN1N | 0.0000 | -84.966 | 188.3 |  |  |