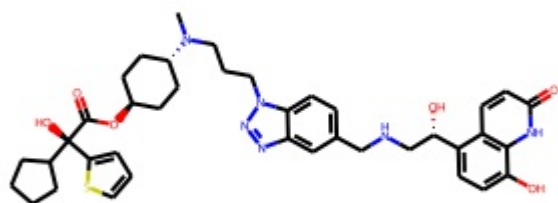
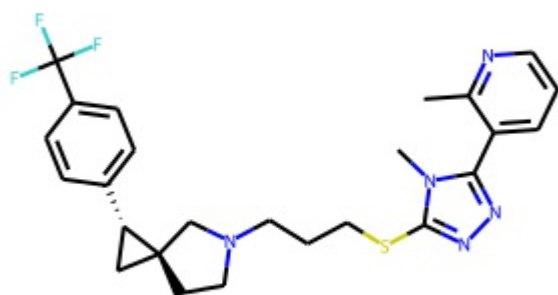


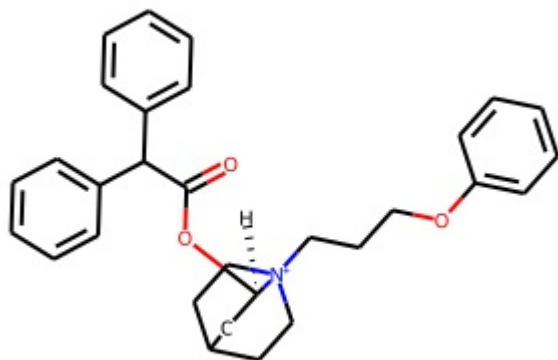
epistemic percentile: 81.8
 p_risky at threshold of 5: [1.]



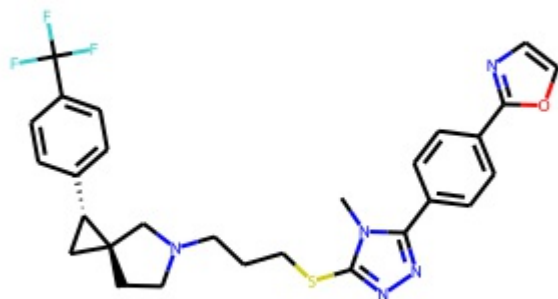
interesting mol: CN(CCCn1nnc2cc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)[C@H]1CC[C@H](OC(=O)[C@](O)(c2cccs2)C2CCCC2)CC1
 predicted mean: [9.39]
 predicted standard deviation: [0.581]
 95% CI: [8.228] - [10.552]
 epistemic percentile: 94.1
 p_risky at threshold of 5: [1.]



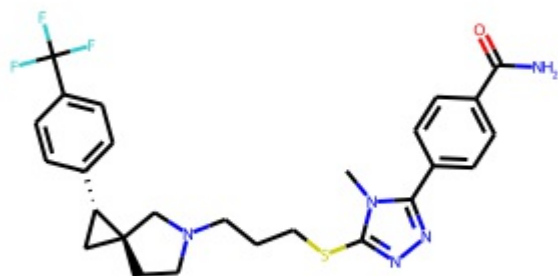
interesting mol: Cc1ncccc1-c1nnc(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)n1C
 predicted mean: [7.219]
 predicted standard deviation: [0.577]
 95% CI: [6.065] - [8.373]
 epistemic percentile: 85.5
 p_risky at threshold of 5: [1.]



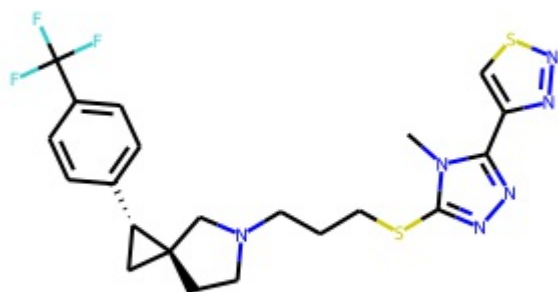
interesting mol: O=C(O[C@@H]1CC2CC[N+]1(CCCOc1ccccc1)CC2)C(c1ccccc1)c1ccccc1
 predicted mean: [7.13]
 predicted standard deviation: [0.525]
 95% CI: [6.081] - [8.18]
 epistemic percentile: 45.1
 p_risky at threshold of 5: [1.]



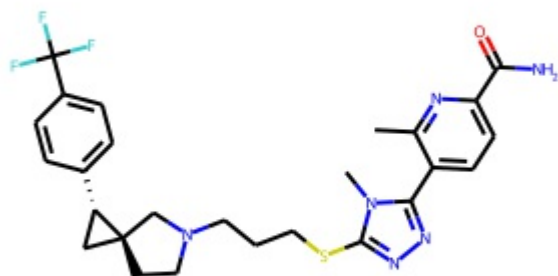
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1-c1ccc(-c2ncco2)cc1
 predicted mean: [6.839]
 predicted standard deviation: [0.595]
 95% CI: [5.648] - [8.03]
 epistemic percentile: 87.0
 p_risky at threshold of 5: [0.999]



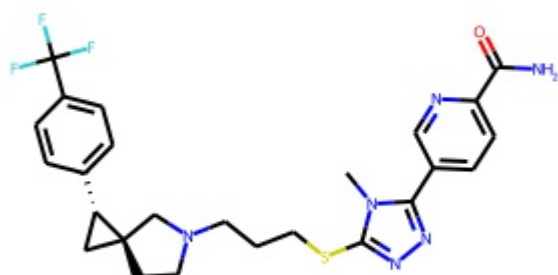
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1-c1ccc(C(N)=O)cc1
 predicted mean: [6.993]
 predicted standard deviation: [0.58]
 95% CI: [5.833] - [8.154]
 epistemic percentile: 84.7
 p_risky at threshold of 5: [1.]



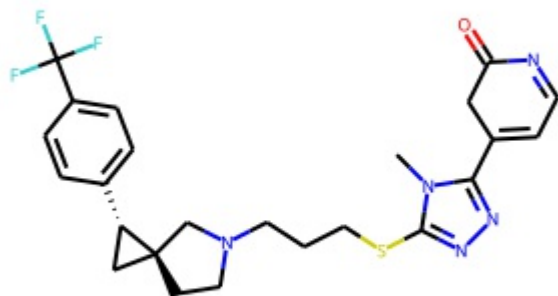
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1-c1csnn1
 predicted mean: [7.077]
 predicted standard deviation: [0.57]
 95% CI: [5.936] - [8.218]
 epistemic percentile: 72.2
 p_risky at threshold of 5: [1.]



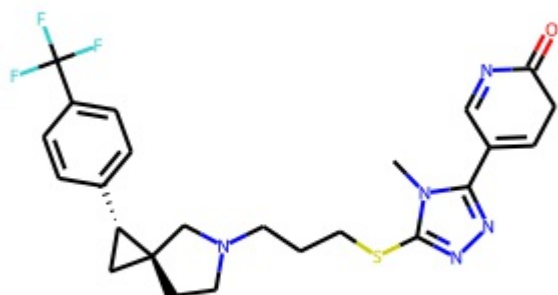
interesting mol: Cc1nc(C(N)=O)ccc1-c1nnc(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)n1C
 predicted mean: [8.06]
 predicted standard deviation: [0.568]
 95% CI: [6.924] - [9.196]
 epistemic percentile: 89.8
 p_risky at threshold of 5: [1.]



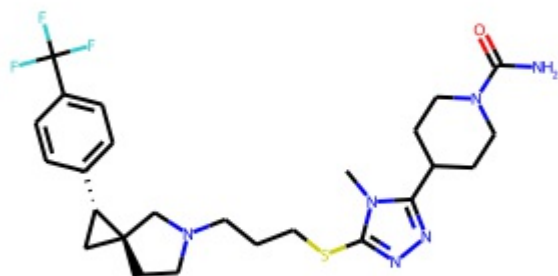
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1-c1ccc(C(N)=O)nc1
 predicted mean: [6.765]
 predicted standard deviation: [0.593]
 95% CI: [5.579] - [7.951]
 epistemic percentile: 83.7
 p_risky at threshold of 5: [0.999]



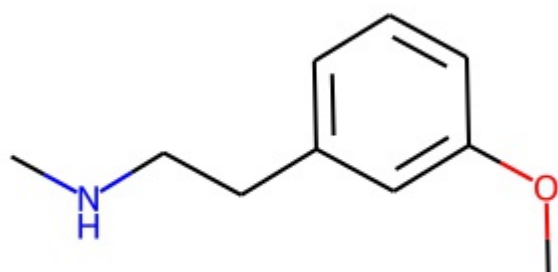
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1C1=CC=NC(=O)C1
 predicted mean: [6.055]
 predicted standard deviation: [0.616]
 95% CI: [4.824] - [7.287]
 epistemic percentile: 73.5
 p_risky at threshold of 5: [0.969]



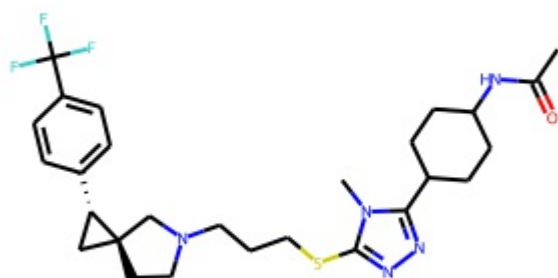
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1C1=CCC(=O)N=C1
 predicted mean: [5.908]
 predicted standard deviation: [0.584]
 95% CI: [4.741] - [7.076]
 epistemic percentile: 70.3
 p_risky at threshold of 5: [0.939]



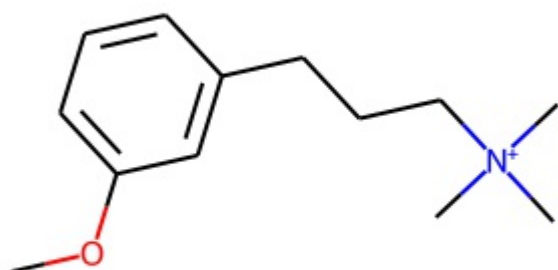
interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1C1CCN(C(N)=O)CC1
 predicted mean: [6.447]
 predicted standard deviation: [0.601]
 95% CI: [5.244] - [7.65]
 epistemic percentile: 84.9
 p_risky at threshold of 5: [0.992]



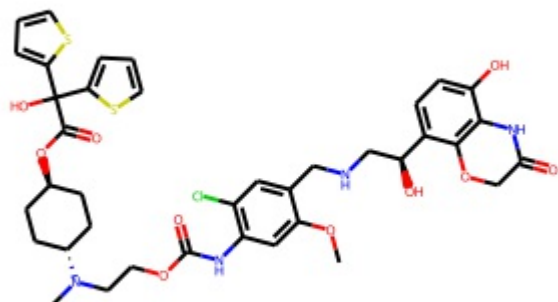
interesting mol: CNCCC1CCCC(OC)C1
 predicted mean: [5.306]
 predicted standard deviation: [0.595]
 95% CI: [4.115] - [6.496]
 epistemic percentile: 24.0
 p_risky at threshold of 5: [0.668]



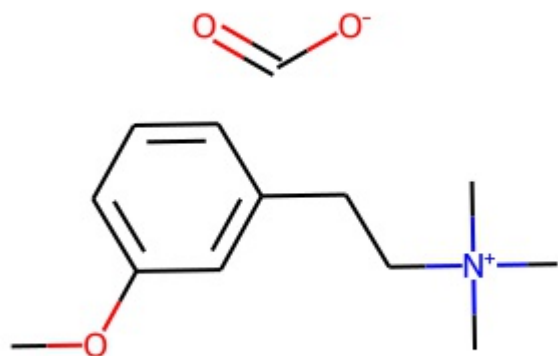
interesting mol: CC(=O)NC1CCC(c2nnc(SCCCN3CC[C@]4(C[C@@H]4c4ccc(C(F)(F)F)cc4)C3)n2C)CC1
 predicted mean: [6.557]
 predicted standard deviation: [0.626]
 95% CI: [5.306] - [7.808]
 epistemic percentile: 90.0
 p_risky at threshold of 5: [0.994]



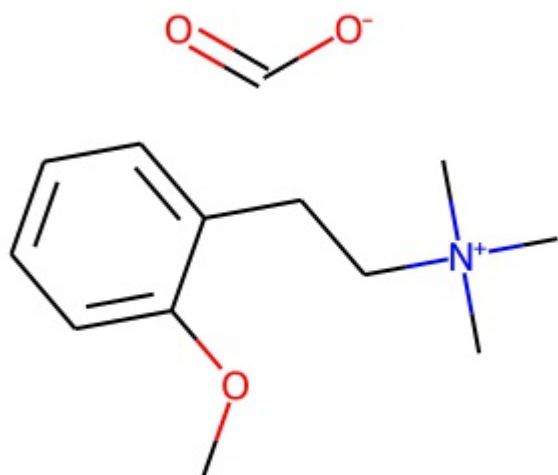
interesting mol: COc1cccc(CCC[N+](C)(C)C)c1
 predicted mean: [6.081]
 predicted standard deviation: [0.566]
 95% CI: [4.95] - [7.213]
 epistemic percentile: 21.4
 p_risky at threshold of 5: [0.965]



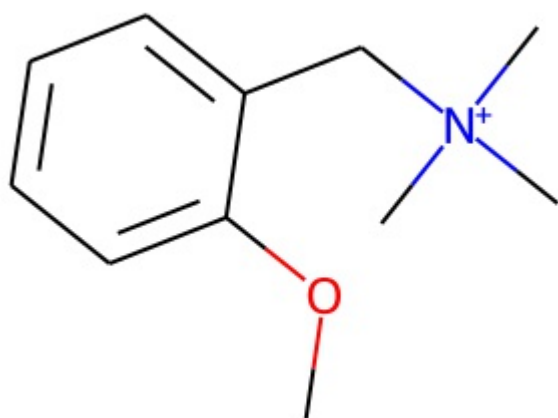
interesting mol: COc1cc(NC(=O)OCCN(C)[C@H]2CC[C@H](OC(=O)C(O)(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2c10CC(=O)N2
 predicted mean: [11.511]
 predicted standard deviation: [0.579]
 95% CI: [10.352] - [12.669]
 epistemic percentile: 99.0
 p_risky at threshold of 5: [1.]



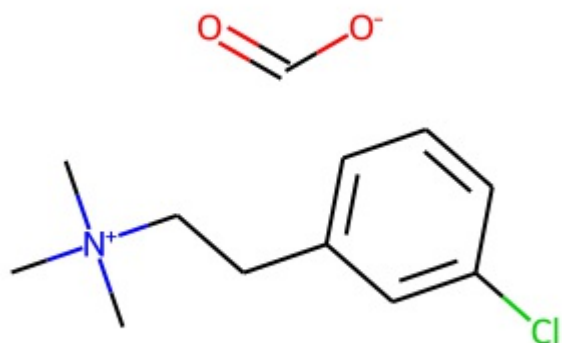
interesting mol: COc1cccc(CC[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [6.34]
 predicted standard deviation: [0.567]
 95% CI: [5.206] - [7.474]
 epistemic percentile: 29.4
 p_risky at threshold of 5: [0.991]



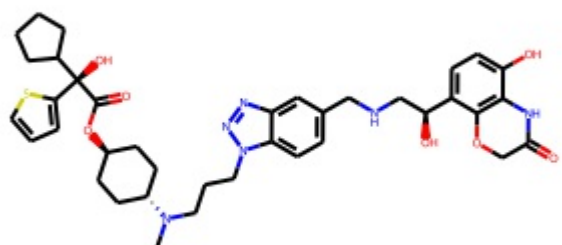
interesting mol: COc1cccc1CC[N+](C)(C)C.O=C[O-]
 predicted mean: [6.21]
 predicted standard deviation: [0.575]
 95% CI: [5.059] - [7.36]
 epistemic percentile: 30.3
 p_risky at threshold of 5: [0.984]



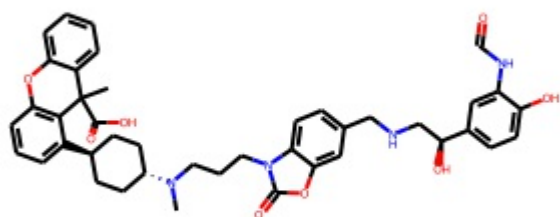
interesting mol: COc1cccc1C[N+](C)(C)C
 predicted mean: [5.299]
 predicted standard deviation: [0.582]
 95% CI: [4.135] - [6.463]
 epistemic percentile: 12.5
 p_risky at threshold of 5: [0.72]



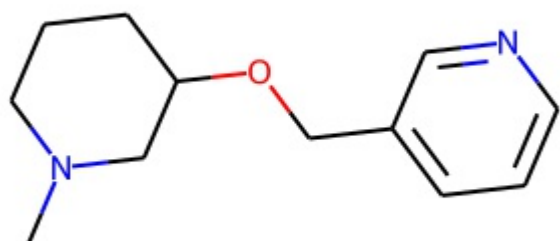
interesting mol: C[N+](C)(C)CCc1ccc(Cl)c1C(=O)[O-]
 predicted mean: [6.413]
 predicted standard deviation: [0.542]
 95% CI: [5.329] - [7.497]
 epistemic percentile: 23.2
 p_risky at threshold of 5: [0.995]



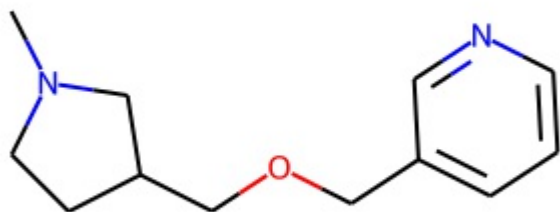
interesting mol: CN(CCCN1N=NC2=CC=C(C=C2)C(=O)N1)C(=O)C3=CC=CC(=O)C4=CC=CC(=O)N4
 predicted mean: [10.332]
 predicted standard deviation: [0.574]
 95% CI: [9.184] - [11.48]
 epistemic percentile: 97.0
 p_risky at threshold of 5: [1.]



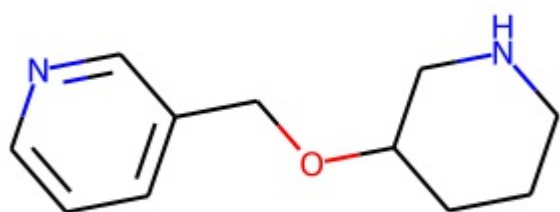
interesting mol: CN(CCCn1c(=O)oc2cc(CNC[C@H](O)c3ccc(O)c(NC=O)c3)ccc21)[C@H]1CC[C@H](c2cccc3c2C(C)(C(=O)O)c2cccc2O3)CC1
 predicted mean: [8.029]
 predicted standard deviation: [0.633]
 95% CI: [6.764] - [9.294]
 epistemic percentile: 96.7
 p_risky at threshold of 5: [1.]



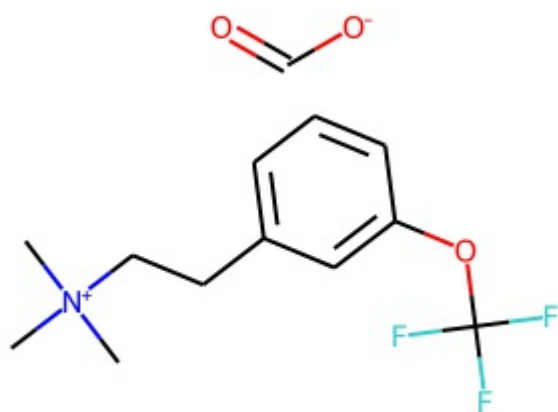
interesting mol: CN1CCCC(OCc2cccnc2)C1
 predicted mean: [6.52]
 predicted standard deviation: [0.567]
 95% CI: [5.385] - [7.654]
 epistemic percentile: 60.8
 p_risky at threshold of 5: [0.997]



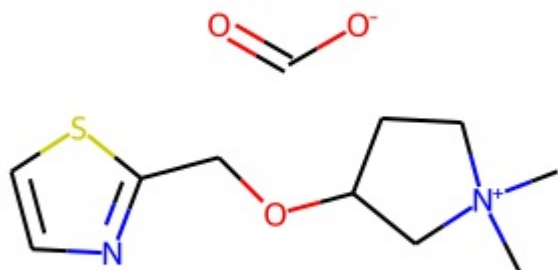
interesting mol: CN1CCC(COCc2ccncc2)C1
 predicted mean: [6.235]
 predicted standard deviation: [0.551]
 95% CI: [5.133] - [7.337]
 epistemic percentile: 35.7
 p_risky at threshold of 5: [0.983]



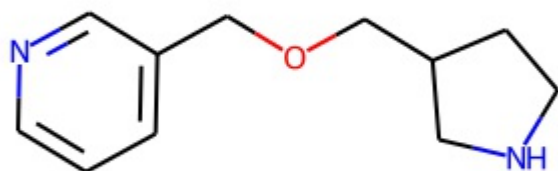
interesting mol: c1cncc(COC2CCCNC2)c1
 predicted mean: [7.169]
 predicted standard deviation: [0.582]
 95% CI: [6.004] - [8.334]
 epistemic percentile: 69.9
 p_risky at threshold of 5: [1.]



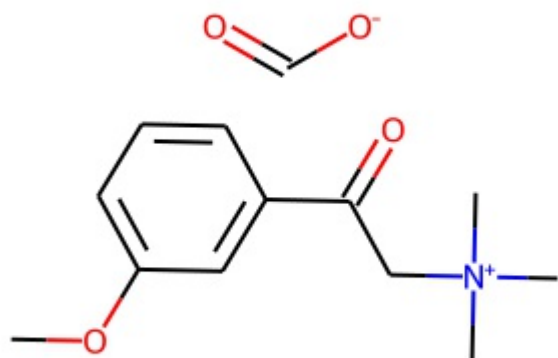
interesting mol: C[N+](C)(C)CCC1CCCC(OC(F)(F)F)C1.O=C[O-]
 predicted mean: [6.041]
 predicted standard deviation: [0.569]
 95% CI: [4.903] - [7.18]
 epistemic percentile: 61.3
 p_risky at threshold of 5: [0.964]



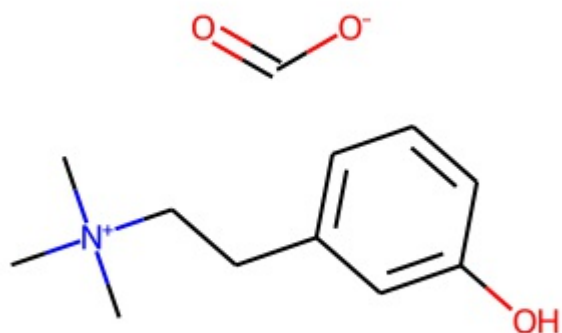
interesting mol: C[N+]1(C)CCC(OCc2nccs2)C1.O=C[O-]
 predicted mean: [7.112]
 predicted standard deviation: [0.563]
 95% CI: [5.987] - [8.238]
 epistemic percentile: 48.8
 p_risky at threshold of 5: [1.]



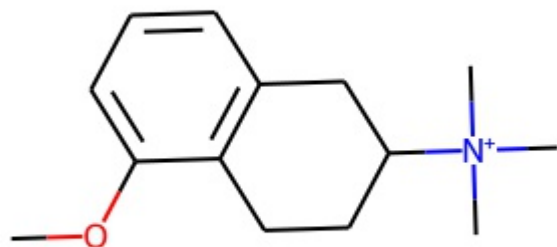
interesting mol: c1cncc(COCC2CCNC2)c1
 predicted mean: [6.335]
 predicted standard deviation: [0.561]
 95% CI: [5.213] - [7.456]
 epistemic percentile: 60.8
 p_risky at threshold of 5: [0.989]



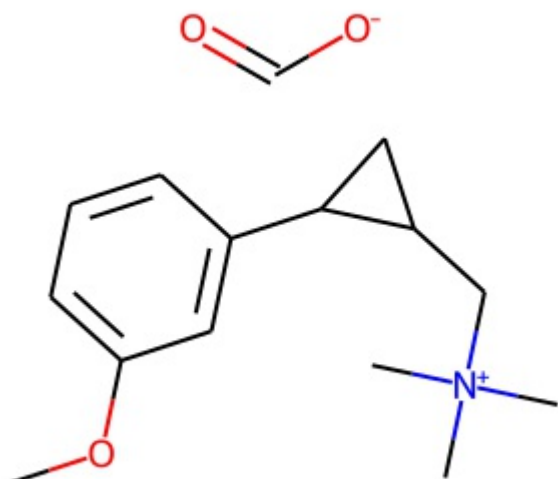
interesting mol: COc1cccc(C(=O)C[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [6.245]
 predicted standard deviation: [0.565]
 95% CI: [5.115] - [7.374]
 epistemic percentile: 14.5
 p_risky at threshold of 5: [0.987]



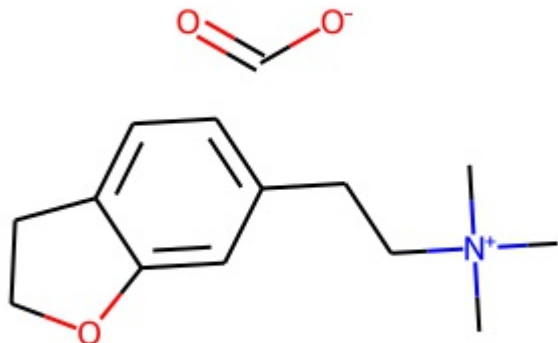
interesting mol: C[N+](C)(C)CCc1cccc(O)c1.O=C[O-]
 predicted mean: [5.617]
 predicted standard deviation: [0.595]
 95% CI: [4.427] - [6.806]
 epistemic percentile: 27.0
 p_risky at threshold of 5: [0.857]



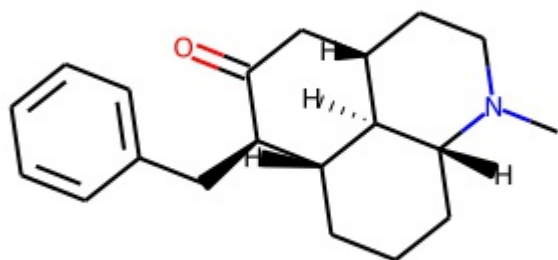
interesting mol: COc1cccc2c1CCC([N+](C)(C)C)C2
 predicted mean: [6.152]
 predicted standard deviation: [0.535]
 95% CI: [5.082] - [7.222]
 epistemic percentile: 6.4
 p_risky at threshold of 5: [0.983]



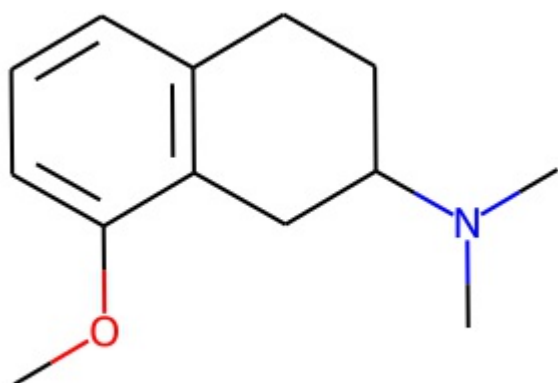
interesting mol: COc1cccc(C2CC2C[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [5.52]
 predicted standard deviation: [0.574]
 95% CI: [4.373] - [6.668]
 epistemic percentile: 19.3
 p_risky at threshold of 5: [0.823]



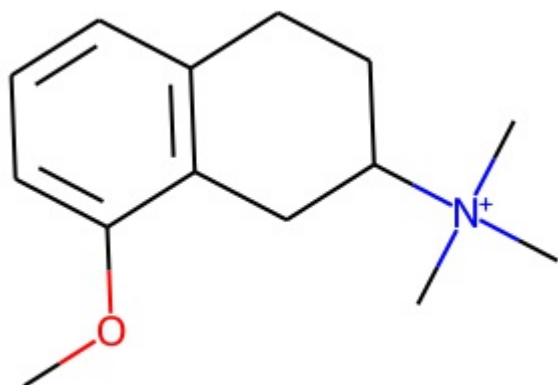
interesting mol: C[N+](C)(C)CCc1ccc2c(c1)OCC2.O=C[O-]
 predicted mean: [5.432]
 predicted standard deviation: [0.586]
 95% CI: [4.259] - [6.604]
 epistemic percentile: 28.4
 p_risky at threshold of 5: [0.807]



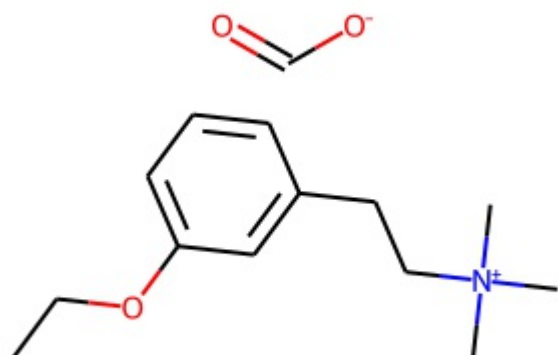
interesting mol: CN1CC[C@H]2CC(=O)[C@H](Cc3ccccc3)[C@H]3CCC[C@@H]1[C@H]23
 predicted mean: [5.079]
 predicted standard deviation: [0.589]
 95% CI: [3.901] - [6.257]
 epistemic percentile: 11.7
 p_risky at threshold of 5: [0.585]



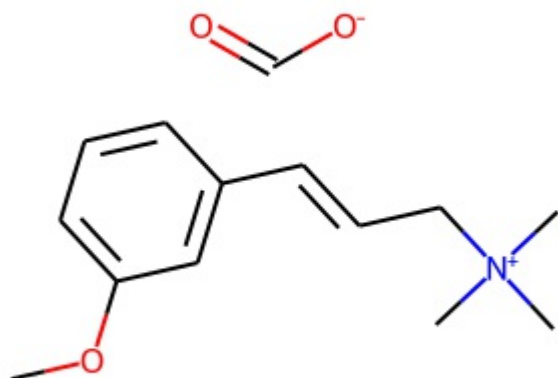
interesting mol: COc1cccc2c1CC(N(C)C)CC2
 predicted mean: [5.99]
 predicted standard deviation: [0.562]
 95% CI: [4.866] - [7.114]
 epistemic percentile: 18.7
 p_risky at threshold of 5: [0.956]



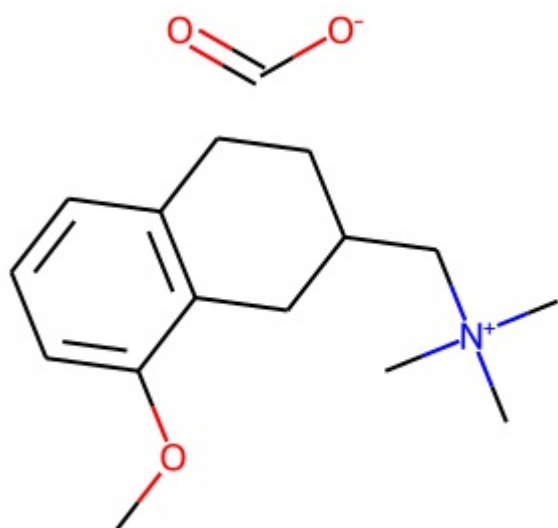
interesting mol: COc1cccc2c1CC([N+](C)(C)C)CC2
 predicted mean: [6.353]
 predicted standard deviation: [0.54]
 95% CI: [5.273] - [7.434]
 epistemic percentile: 10.4
 p_risky at threshold of 5: [0.993]



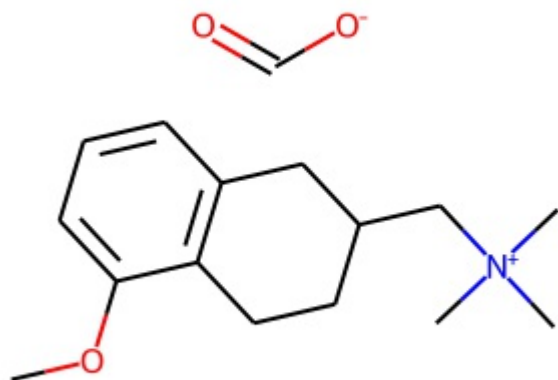
interesting mol: CCOc1cccc(CC[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [5.932]
 predicted standard deviation: [0.583]
 95% CI: [4.766] - [7.098]
 epistemic percentile: 31.2
 p_risky at threshold of 5: [0.954]



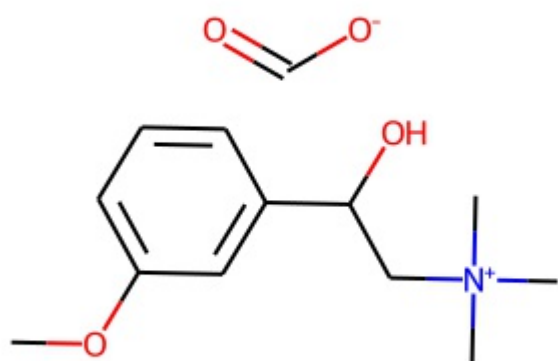
interesting mol: COC1CCCC(/C=C/C[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [5.693]
 predicted standard deviation: [0.567]
 95% CI: [4.558] - [6.828]
 epistemic percentile: 14.6
 p_risky at threshold of 5: [0.895]



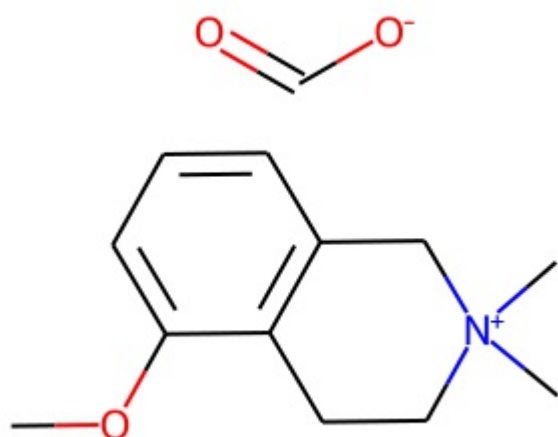
interesting mol: COC1CCCC2C1CC(C[N+](C)(C)C)CC2.O=C[O-]
 predicted mean: [7.112]
 predicted standard deviation: [0.55]
 95% CI: [6.013] - [8.212]
 epistemic percentile: 36.2
 p_risky at threshold of 5: [1.]



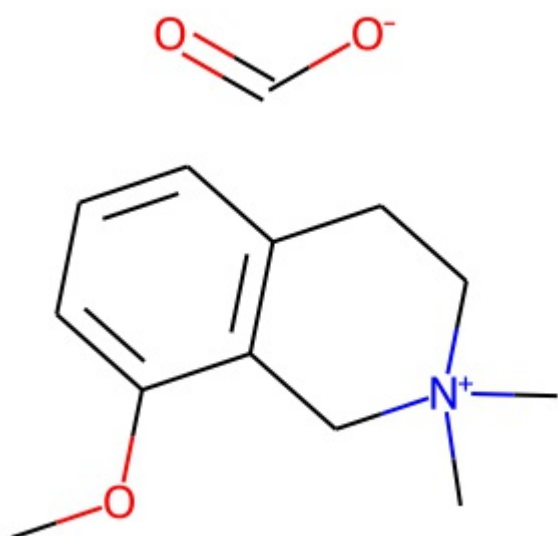
interesting mol: COc1cccc2c1CCC(C[N+](C)(C)C)C2.O=C[O-]
 predicted mean: [7.115]
 predicted standard deviation: [0.546]
 95% CI: [6.023] - [8.207]
 epistemic percentile: 33.3
 p_risky at threshold of 5: [1.]



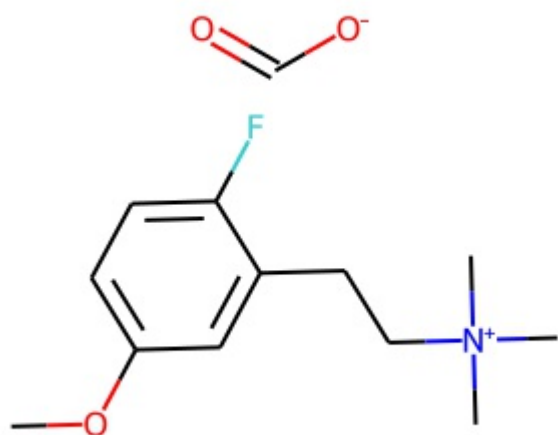
interesting mol: COc1cccc(C(O)C[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [6.652]
 predicted standard deviation: [0.562]
 95% CI: [5.528] - [7.776]
 epistemic percentile: 27.9
 p_risky at threshold of 5: [0.999]



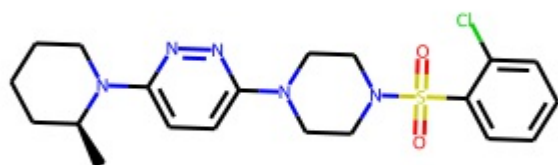
interesting mol: COC1CCCC2C1CC[N+](C)(C)C2.O=C[O-]
 predicted mean: [6.197]
 predicted standard deviation: [0.549]
 95% CI: [5.098] - [7.296]
 epistemic percentile: 14.2
 p_risky at threshold of 5: [0.984]



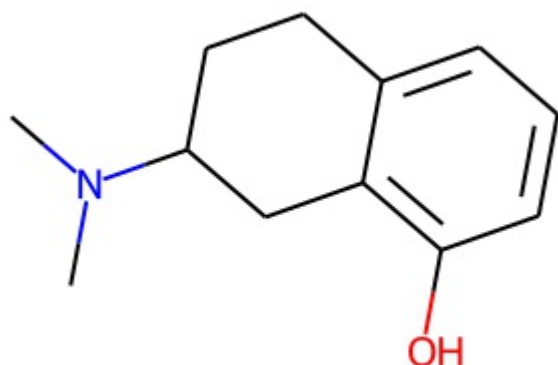
interesting mol: COC1CCCC2C1C[N+](C)(C)CC2.O=C[O-]
 predicted mean: [6.117]
 predicted standard deviation: [0.574]
 95% CI: [4.969] - [7.265]
 epistemic percentile: 17.6
 p_risky at threshold of 5: [0.976]



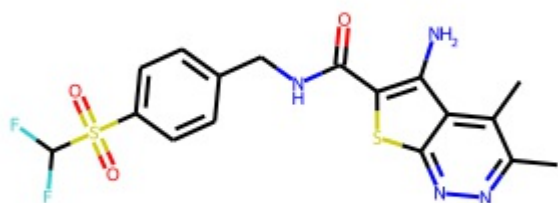
interesting mol: COc1ccc(F)c(CC[N+](C)(C)C)c1.O=C[O-]
 predicted mean: [6.609]
 predicted standard deviation: [0.56]
 95% CI: [5.489] - [7.729]
 epistemic percentile: 36.1
 p_risky at threshold of 5: [0.998]



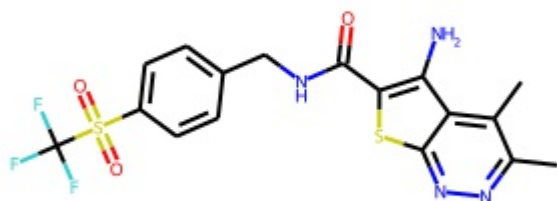
interesting mol: C[C@H]1CCCCN1c1ccc(N2CCN(S(=O)(=O)c3ccccc3Cl)CC2)nn1
 predicted mean: [6.543]
 predicted standard deviation: [0.551]
 95% CI: [5.441] - [7.644]
 epistemic percentile: 36.9
 p_risky at threshold of 5: [0.998]



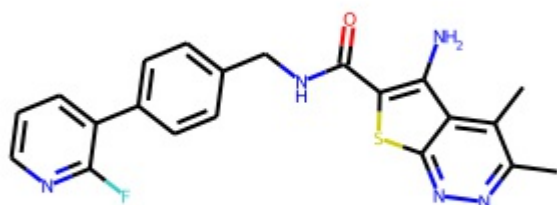
interesting mol: CN(C)C1CCc2cccc(O)c2C1
 predicted mean: [5.455]
 predicted standard deviation: [0.569]
 95% CI: [4.317] - [6.594]
 epistemic percentile: 9.5
 p_risky at threshold of 5: [0.759]



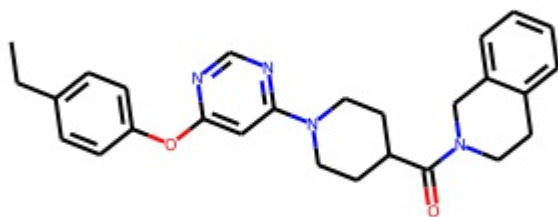
interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(S(=O)(=O)C(F)F)cc3)c(N)c2c1C
 predicted mean: [5.858]
 predicted standard deviation: [0.563]
 95% CI: [4.732] - [6.983]
 epistemic percentile: 44.5
 p_risky at threshold of 5: [0.931]



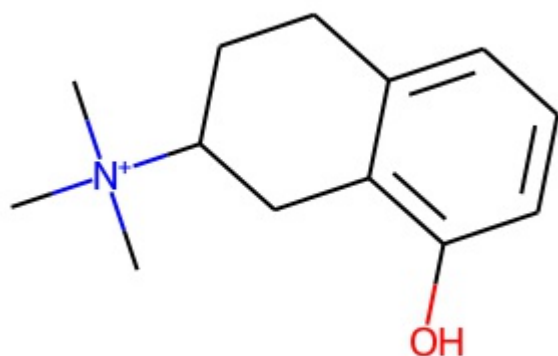
interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(S(=O)(=O)C(F)(F)F)cc3)c(N)c2c1C
 predicted mean: [5.498]
 predicted standard deviation: [0.589]
 95% CI: [4.32] - [6.675]
 epistemic percentile: 38.1
 p_risky at threshold of 5: [0.821]



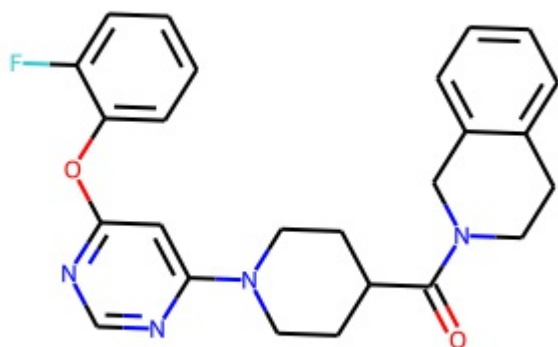
interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(-c4cccncc4F)cc3)c(N)c2c1C
 predicted mean: [6.32]
 predicted standard deviation: [0.598]
 95% CI: [5.125] - [7.516]
 epistemic percentile: 86.5
 p_risky at threshold of 5: [0.986]



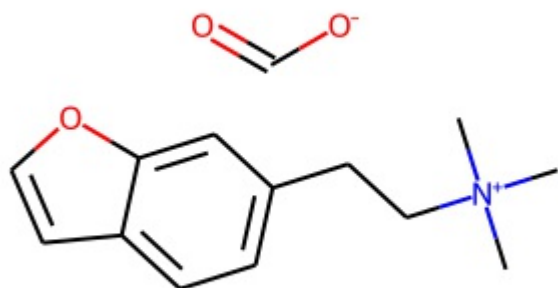
interesting mol: CCc1ccc(Oc2cc(N3CCC(C(=O)N4CCc5ccccc5C4)CC3)ncn2)cc1
 predicted mean: [4.712]
 predicted standard deviation: [0.621]
 95% CI: [3.471] - [5.954]
 epistemic percentile: 43.7
 p_risky at threshold of 5: [0.341]



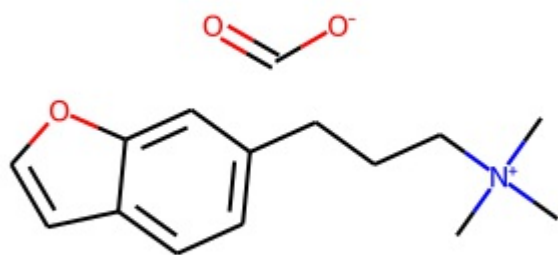
interesting mol: C[N+](C)(C)C1CCc2cc(O)c(C1)cc2
 predicted mean: [5.836]
 predicted standard deviation: [0.537]
 95% CI: [4.763] - [6.91]
 epistemic percentile: 7.6
 p_risky at threshold of 5: [0.929]



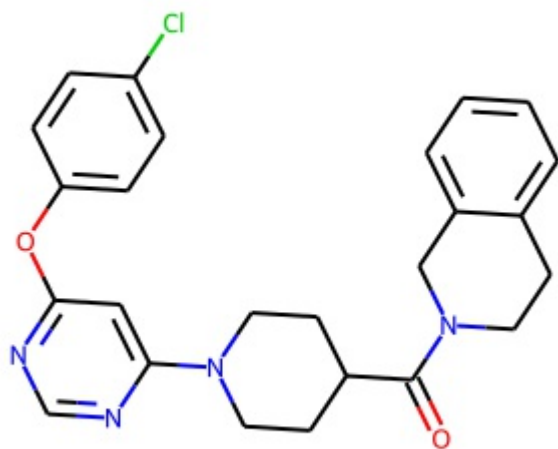
interesting mol: O=C(C1CCN(c2cc(oc3ccccc3F)ncn2)CC1)N1CCc2ccccc2C1
 predicted mean: [6.253]
 predicted standard deviation: [0.58]
 95% CI: [5.093] - [7.413]
 epistemic percentile: 53.4
 p_risky at threshold of 5: [0.983]



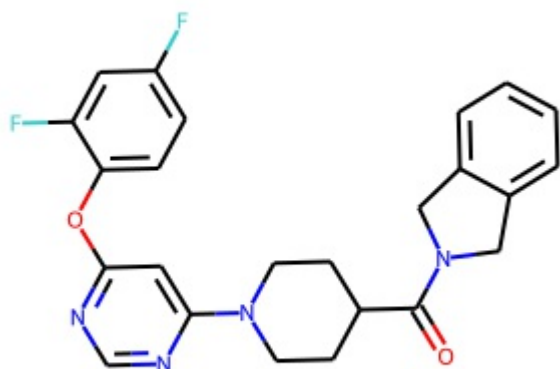
interesting mol: C[N+](C)(C)CCc1ccc2ccoc2c1.O=C[O-]
 predicted mean: [5.043]
 predicted standard deviation: [0.585]
 95% CI: [3.874] - [6.213]
 epistemic percentile: 41.6
 p_risky at threshold of 5: [0.524]



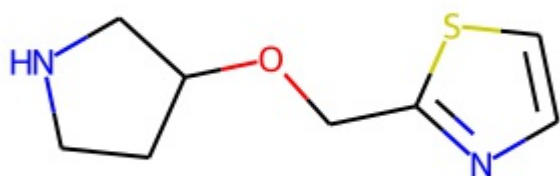
interesting mol: C[N+](C)(C)CCCc1ccc2ccoc2c1.O=C[O-]
 predicted mean: [5.1]
 predicted standard deviation: [0.592]
 95% CI: [3.915] - [6.285]
 epistemic percentile: 43.0
 p_risky at threshold of 5: [0.585]



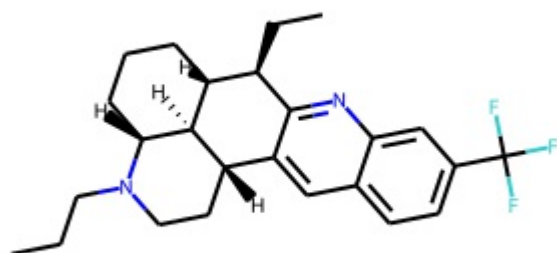
interesting mol: O=C(C1CCN(c2cc(oc3ccc(Cl)cc3)ncn2)CC1)N1CCc2ccccc2C1
 predicted mean: [6.084]
 predicted standard deviation: [0.597]
 95% CI: [4.891] - [7.277]
 epistemic percentile: 54.0
 p_risky at threshold of 5: [0.966]



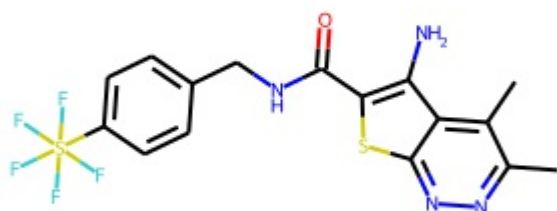
interesting mol: O=C(C1CCN(c2cc(oc3ccc(F)cc3F)ncn2)CC1)N1Cc2ccccc2C1
 predicted mean: [5.273]
 predicted standard deviation: [0.597]
 95% CI: [4.08] - [6.467]
 epistemic percentile: 46.8
 p_risky at threshold of 5: [0.675]



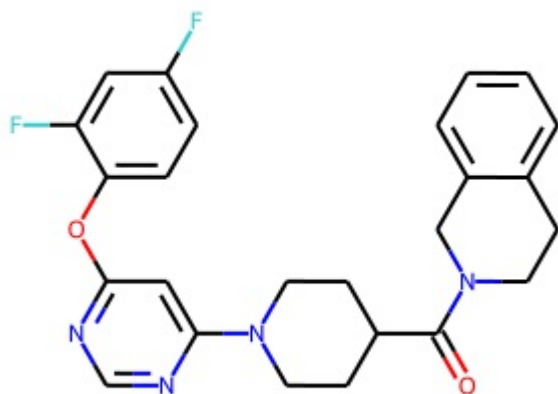
interesting mol: c1csc(COC2CCNC2)n1
 predicted mean: [7.041]
 predicted standard deviation: [0.539]
 95% CI: [5.963] - [8.12]
 epistemic percentile: 39.8
 p_risky at threshold of 5: [1.]



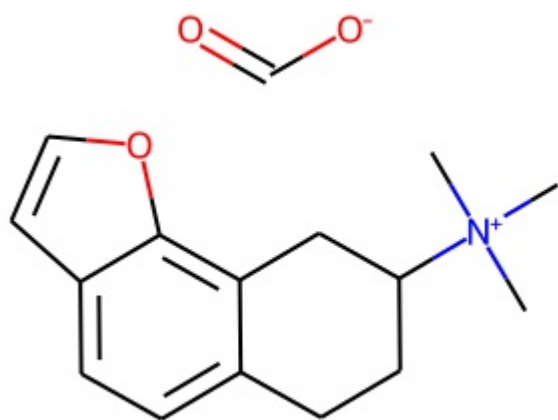
interesting mol: CCCN1CC[C@H]2c3cc4ccc(C(F)(F)F)cc4nc3[C@H](CC)[C@H]3CCC[C@@H]1[C@@H]32
 predicted mean: [5.303]
 predicted standard deviation: [0.633]
 95% CI: [4.037] - [6.569]
 epistemic percentile: 65.5
 p_risky at threshold of 5: [0.671]



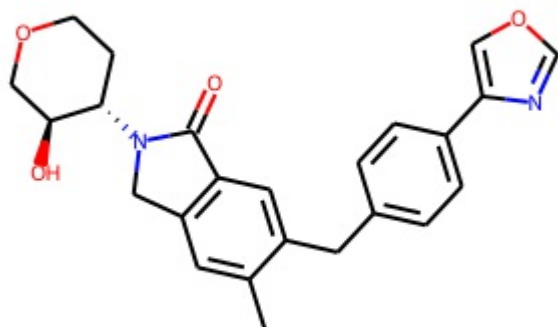
interesting mol: Cc1nnc2sc(C(=O)NCC3ccc(S(F)(F)(F)F)cc3)c(N)c2c1C
 predicted mean: [5.304]
 predicted standard deviation: [0.588]
 95% CI: [4.128] - [6.48]
 epistemic percentile: 48.3
 p_risky at threshold of 5: [0.695]



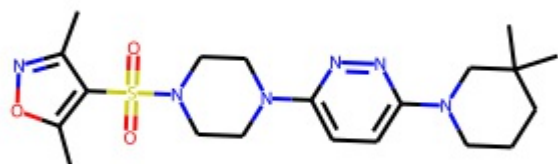
interesting mol: O=C(C1CCN(c2cc(oc3ccc(F)cc3F)ncn2)CC1)N1CCc2ccccc2C1
 predicted mean: [5.681]
 predicted standard deviation: [0.596]
 95% CI: [4.488] - [6.873]
 epistemic percentile: 61.3
 p_risky at threshold of 5: [0.881]



interesting mol: C[N+](C)(C)C1CCc2ccc3ccoc3c2C1.O=C[O-]
 predicted mean: [5.479]
 predicted standard deviation: [0.575]
 95% CI: [4.328] - [6.629]
 epistemic percentile: 24.0
 p_risky at threshold of 5: [0.823]



interesting mol: Cc1cc2c(cc1Cc1ccc(-c3cocn3)cc1)C(=O)N([C@H]1CCOC[C@H]1O)C2
 predicted mean: [5.528]
 predicted standard deviation: [0.583]
 95% CI: [4.361] - [6.694]
 epistemic percentile: 57.0
 p_risky at threshold of 5: [0.804]



interesting mol: Cc1noc(C)c1S(=O)(=O)N1CCN(c2ccc(N3CCCC(C)(C)C3)nn2)CC1
 predicted mean: [6.152]
 predicted standard deviation: [0.577]
 95% CI: [4.999] - [7.306]
 epistemic percentile: 43.0
 p_risky at threshold of 5: [0.98]

In [2]: