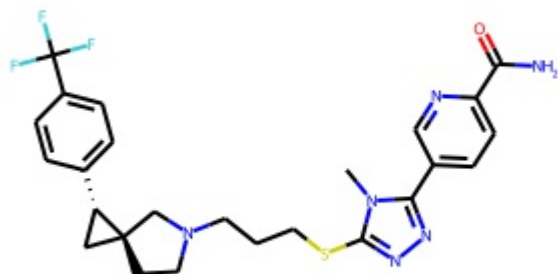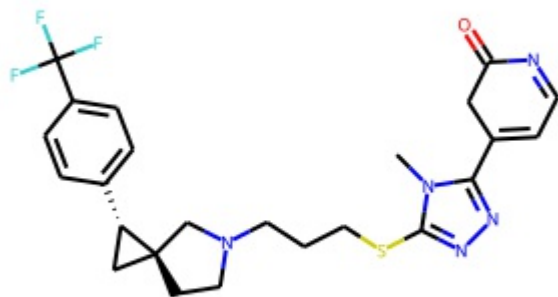aleatoric uncertainty: [0.42]
epistemic uncertainty: [0.341]
p_risky at threshold of 5: [0.]

interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1-c1ccc(C(N)=O)nc1
predicted mean: [7.462]
predicted standard deviation: [0.576]
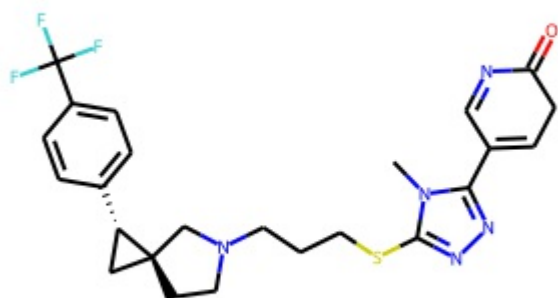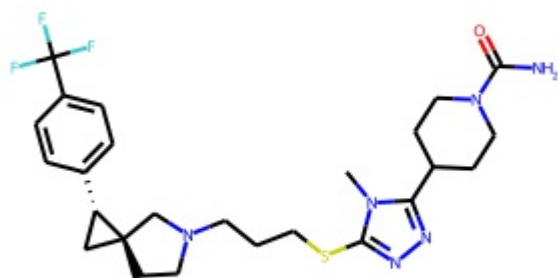95% CI: [6.311] - [8.614]
aleatoric uncertainty: [0.425]
epistemic uncertainty: [0.339]
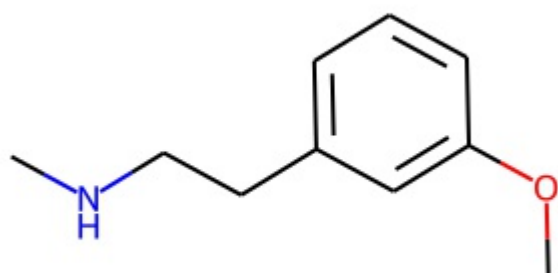p_risky at threshold of 5: [0.]

interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)(F)F)cc3)C2)nnc1C1=CC=NC(=O)C1
predicted mean: [5.813]
predicted standard deviation: [0.567]
95% CI: [4.678] - [6.947]
aleatoric uncertainty: [0.476]
epistemic uncertainty: [0.316]
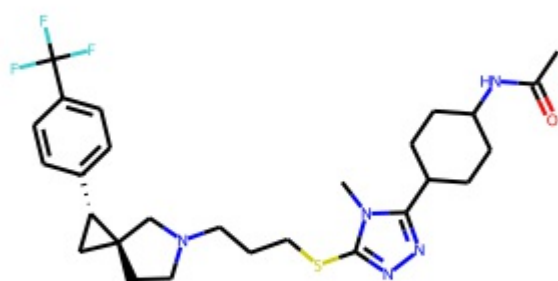p_risky at threshold of 5: [0.084]

interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)
(F)F)cc3)C2)nnc1C1=CCC(=O)N=C1
predicted mean: [5.116]
predicted standard deviation: [0.584]
95% CI: [3.948] - [6.285]
aleatoric uncertainty: [0.501]
epistemic uncertainty: [0.297]
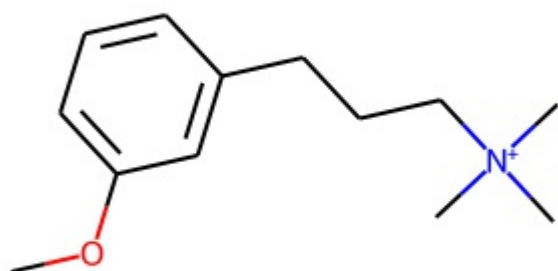p_risky at threshold of 5: [0.421]

interesting mol: Cn1c(SCCCN2CC[C@]3(C[C@@H]3c3ccc(C(F)
(F)F)cc3)C2)nnc1C1CCN(C(N)=O)CC1
predicted mean: [6.84]
predicted standard deviation: [0.566]
95% CI: [5.707] - [7.972]
aleatoric uncertainty: [0.443]
epistemic uncertainty: [0.345]
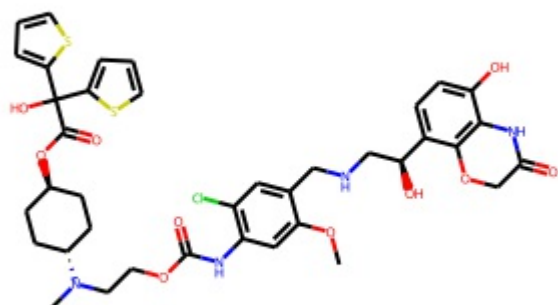p_risky at threshold of 5: [0.]

interesting mol: CNCCc1cccc(OC)c1
predicted mean: [5.55]
predicted standard deviation: [0.546]
95% CI: [4.458] - [6.642]
aleatoric uncertainty: [0.486]
epistemic uncertainty: [0.257]
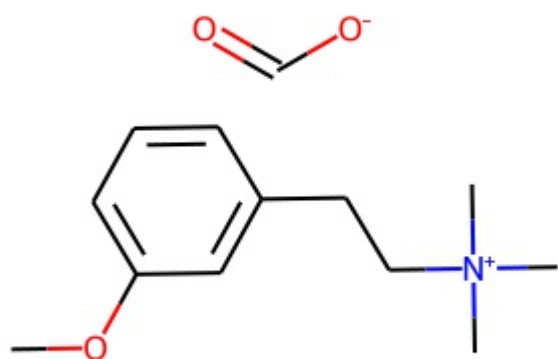p_risky at threshold of 5: [0.15]

interesting mol: CC(=O)NC1CCC(c2nnc(SCCCN3CC[C@]4(C[C@@H]4c4ccc(C(F)(F)F)cc4)C3)n2C)CC1
predicted mean: [6.447]
predicted standard deviation: [0.575]
95% CI: [5.297] - [7.598]
aleatoric uncertainty: [0.453]
epistemic uncertainty: [0.352]
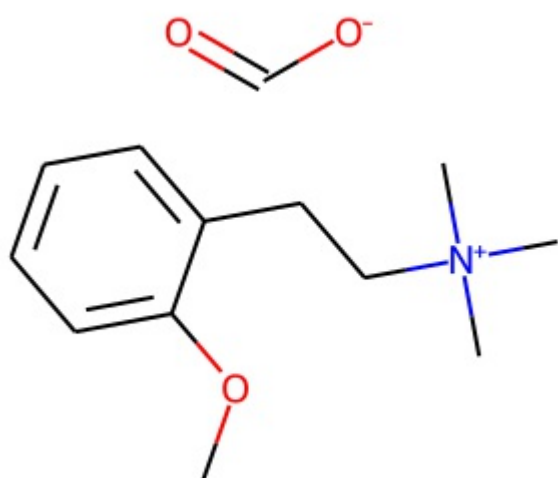p_risky at threshold of 5: [0.007]

interesting mol: COc1cccc(CCC[N+](C)(C)C)c1
predicted mean: [5.456]
predicted standard deviation: [0.543]
95% CI: [4.369] - [6.543]
aleatoric uncertainty: [0.492]
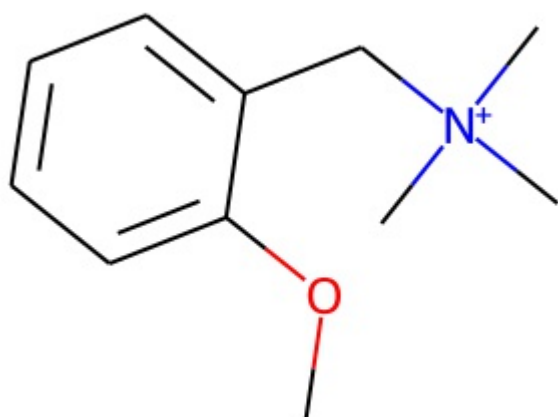epistemic uncertainty: [0.227]
p_risky at threshold of 5: [0.217]

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)c2c1OCC(=O)N2
predicted mean: [10.581]
predicted standard deviation: [0.584]
95% CI: [9.414] - [11.748]
aleatoric uncertainty: [0.33]
epistemic uncertainty: [0.489]
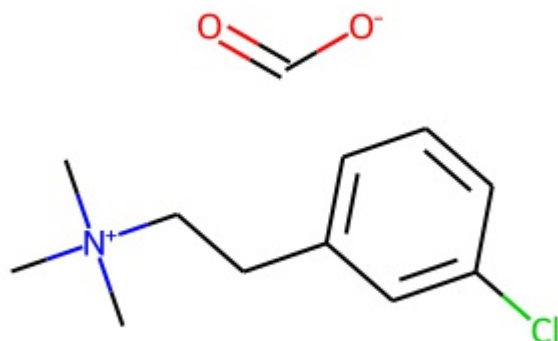p_risky at threshold of 5: [0.]

interesting mol: COc1cccc(CC[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.504]
predicted standard deviation: [0.548]
95% CI: [4.408] - [6.6]
aleatoric uncertainty: [0.492]
epistemic uncertainty: [0.256]
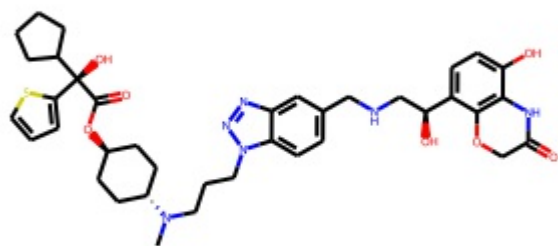p_risky at threshold of 5: [0.19]

interesting mol: COc1ccccc1CC[N+](C)(C)C.O=C[O-]
predicted mean: [4.62]
predicted standard deviation: [0.605]
95% CI: [3.41] - [5.829]
aleatoric uncertainty: [0.521]
epistemic uncertainty: [0.239]
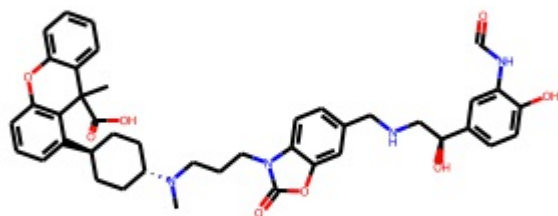p_risky at threshold of 5: [0.71]

interesting mol: COc1ccccc1C[N+](C)(C)C
predicted mean: [4.4]
predicted standard deviation: [0.55]
95% CI: [3.3] - [5.5]
aleatoric uncertainty: [0.526]
epistemic uncertainty: [0.233]
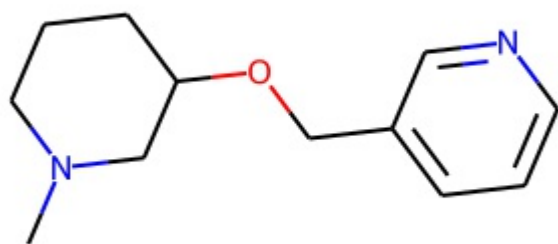p_risky at threshold of 5: [0.811]

interesting mol: C[N+](C)(C)CCc1cccc(Cl)c1.O=C[O-]
predicted mean: [5.994]
predicted standard deviation: [0.519]
95% CI: [4.955] - [7.032]
aleatoric uncertainty: [0.475]
epistemic uncertainty: [0.227]
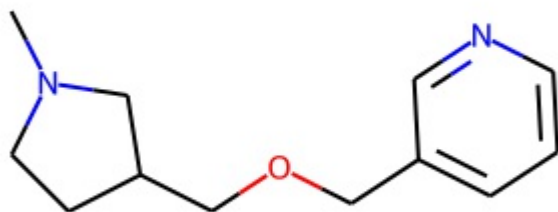p_risky at threshold of 5: [0.02]

interesting mol: CN(CCCn1nnc2cc(CNC[C@H](O)c3ccc(O)c4c3OCC(=O)N4)ccc21)
[C@H]1CC[C@H](OC(=O)[C@](O)(c2cccs2)C2CCCC2)CC1
predicted mean: [10.764]
predicted standard deviation: [0.49]
95% CI: [9.784] - [11.743]
aleatoric uncertainty: [0.329]
epistemic uncertainty: [0.376]
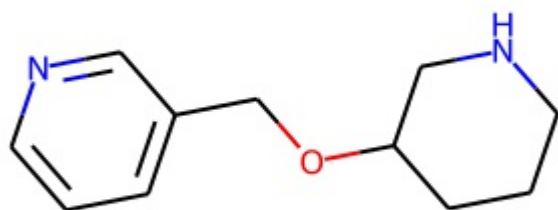p_risky at threshold of 5: [0.]

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)c2ccccc2O3)CC1
predicted mean: [8.283]
predicted standard deviation: [0.657]
95% CI: [6.969] - [9.597]
aleatoric uncertainty: [0.398]
epistemic uncertainty: [0.518]
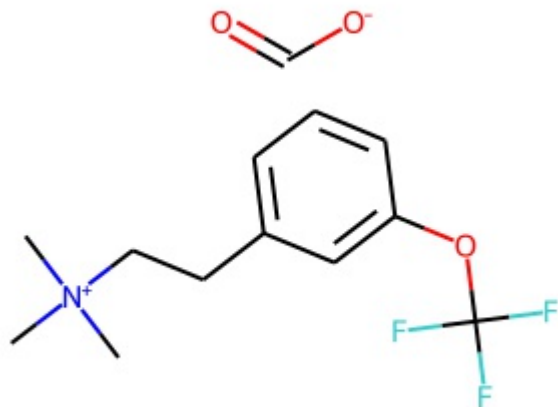p_risky at threshold of 5: [0.]

interesting mol: CN1CCCC(OCc2cccnc2)C1
predicted mean: [5.812]
predicted standard deviation: [0.543]
95% CI: [4.726] - [6.897]
aleatoric uncertainty: [0.481]
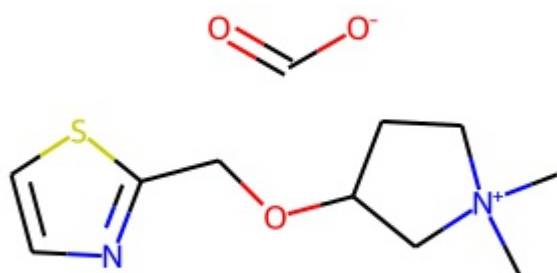epistemic uncertainty: [0.249]
p_risky at threshold of 5: [0.079]

interesting mol: CN1CCC(COCc2cccnc2)C1
predicted mean: [5.716]
predicted standard deviation: [0.521]
95% CI: [4.674] - [6.758]
aleatoric uncertainty: [0.485]
epistemic uncertainty: [0.205]
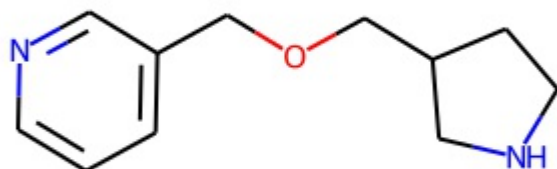p_risky at threshold of 5: [0.097]

```
interesting mol: c1cncc(COC2CCCNC2)c1
predicted mean: [6.744]
predicted standard deviation: [0.535]
95% CI: [5.673] - [7.815]
aleatoric uncertainty: [0.445]
epistemic uncertainty: [0.295]
p_risky at threshold of 5: [0.001]
```
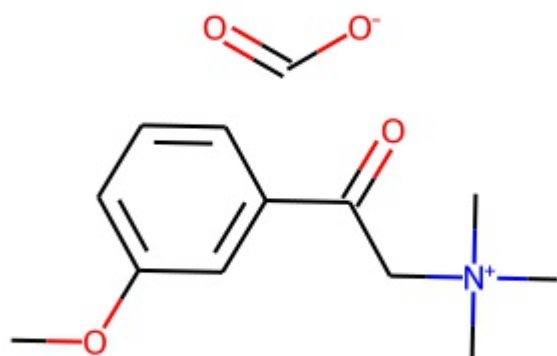


```
interesting mol: C[N+](C)(C)CCc1cccc(OC(F)(F)F)c1.O=C[O-]
predicted mean: [4.97]
predicted standard deviation: [0.565]
95% CI: [3.839] - [6.1]
aleatoric uncertainty: [0.51]
epistemic uncertainty: [0.285]
p_risky at threshold of 5: [0.487]
```
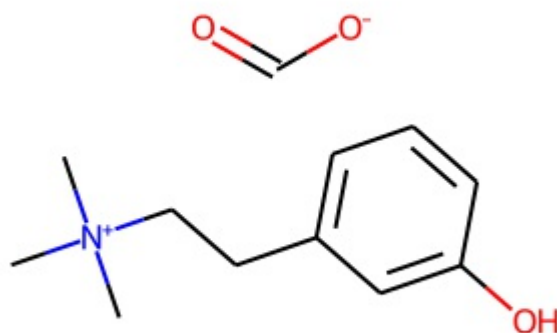
interesting mol: C[N+]1(C)CCC(OCc2nccs2)C1.O=C[O-]
predicted mean: [6.559]
predicted standard deviation: [0.511]
95% CI: [5.537] - [7.58]
aleatoric uncertainty: [0.455]
epistemic uncertainty: [0.234]
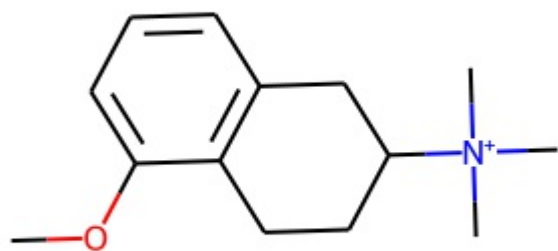p_risky at threshold of 5: [0.001]

interesting mol: c1cncc(COCC2CCNC2)c1
predicted mean: [5.344]
predicted standard deviation: [0.551]
95% CI: [4.241] - [6.447]
aleatoric uncertainty: [0.495]
epistemic uncertainty: [0.265]
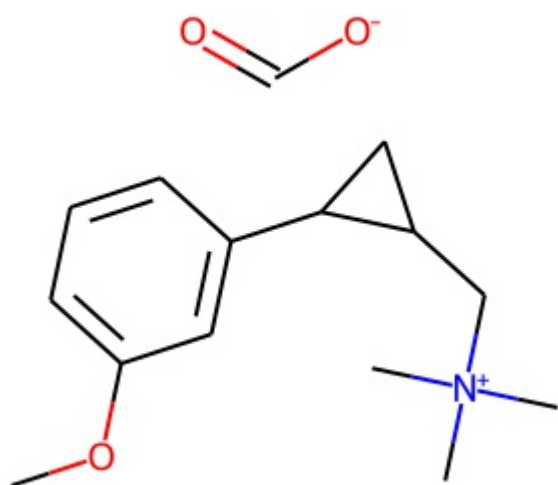p_risky at threshold of 5: [0.249]

interesting mol: COc1cccc(C(=O)C[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.543]
predicted standard deviation: [0.54]
95% CI: [4.464] - [6.622]
aleatoric uncertainty: [0.489]
epistemic uncertainty: [0.24]
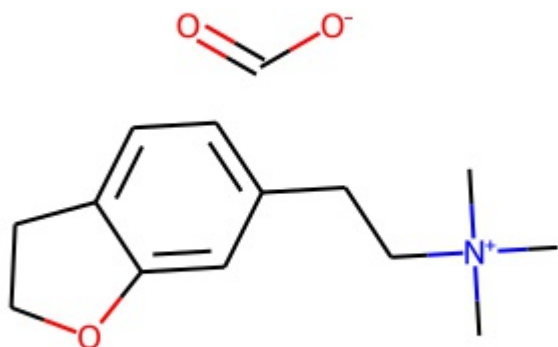p_risky at threshold of 5: [0.147]

interesting mol: C[N+](C)(C)CCc1cccc(O)c1.O=C[O-]
predicted mean: [5.691]
predicted standard deviation: [0.522]
95% CI: [4.646] - [6.736]
aleatoric uncertainty: [0.485]
epistemic uncertainty: [0.245]
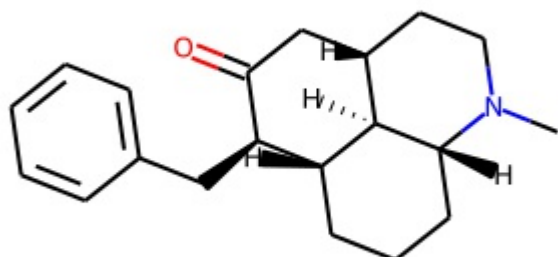p_risky at threshold of 5: [0.099]

interesting mol: COc1cccc2c1CCC([N+](C)(C)C)C2
predicted mean: [5.839]
predicted standard deviation: [0.506]
95% CI: [4.828] - [6.851]
aleatoric uncertainty: [0.48]
epistemic uncertainty: [0.169]
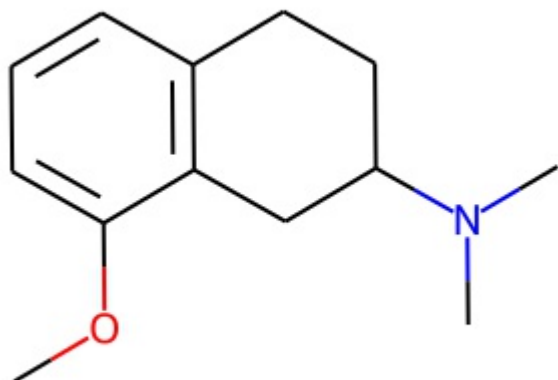p_risky at threshold of 5: [0.054]

interesting mol: COc1cccc(C2CC2C[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.194]
predicted standard deviation: [0.569]
95% CI: [4.056] - [6.332]
aleatoric uncertainty: [0.503]
epistemic uncertainty: [0.195]
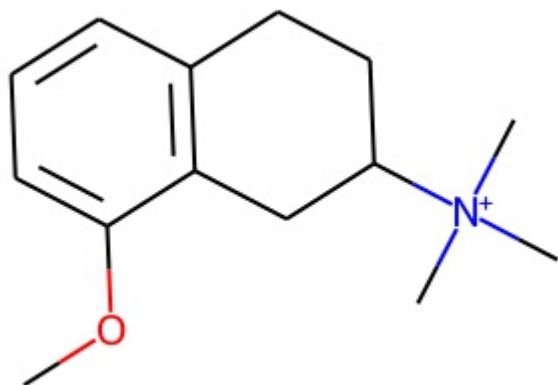p_risky at threshold of 5: [0.362]

interesting mol: C[N+](C)(C)CCc1ccc2c(c1)OCC2.O=C[O-]
predicted mean: [5.585]
predicted standard deviation: [0.536]
95% CI: [4.512] - [6.657]
aleatoric uncertainty: [0.487]
epistemic uncertainty: [0.239]
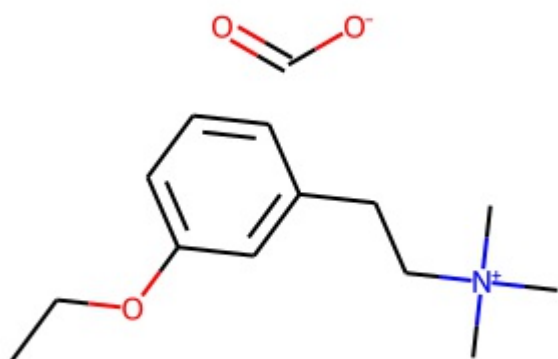p_risky at threshold of 5: [0.141]

interesting mol: CN1CC[C@H]2CC(=O)[C@H](Cc3ccccc3)[C@H]3CCC[C@@H]1[C@H]23
predicted mean: [5.252]
predicted standard deviation: [0.562]
95% CI: [4.128] - [6.375]
aleatoric uncertainty: [0.498]
epistemic uncertainty: [0.216]
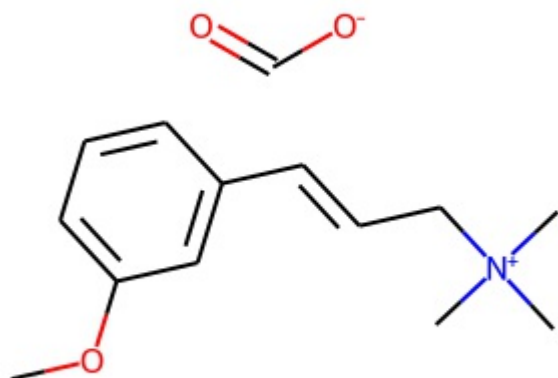p_risky at threshold of 5: [0.297]

interesting mol: COc1cccc2c1CC(N(C)C)CC2
predicted mean: [5.036]
predicted standard deviation: [0.568]
95% CI: [3.9] - [6.172]
aleatoric uncertainty: [0.508]
epistemic uncertainty: [0.192]
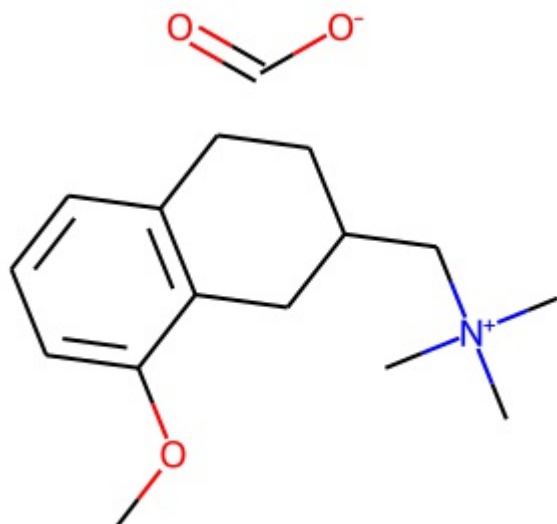p_risky at threshold of 5: [0.502]

interesting mol: COc1cccc2c1CC([N+](C)(C)C)CC2
predicted mean: [5.481]
predicted standard deviation: [0.556]
95% CI: [4.37] - [6.592]
aleatoric uncertainty: [0.493]
epistemic uncertainty: [0.191]
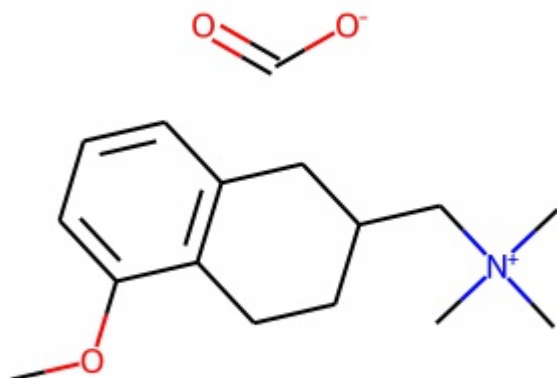p_risky at threshold of 5: [0.185]

interesting mol: CCOc1cccc(CC[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.48]
predicted standard deviation: [0.543]
95% CI: [4.394] - [6.566]
aleatoric uncertainty: [0.492]
epistemic uncertainty: [0.271]
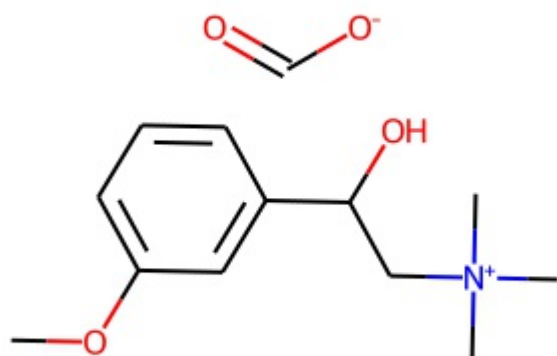p_risky at threshold of 5: [0.185]

interesting mol: COc1cccc(/C=C/C[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.178]
predicted standard deviation: [0.548]
95% CI: [4.083] - [6.274]
aleatoric uncertainty: [0.503]
epistemic uncertainty: [0.213]
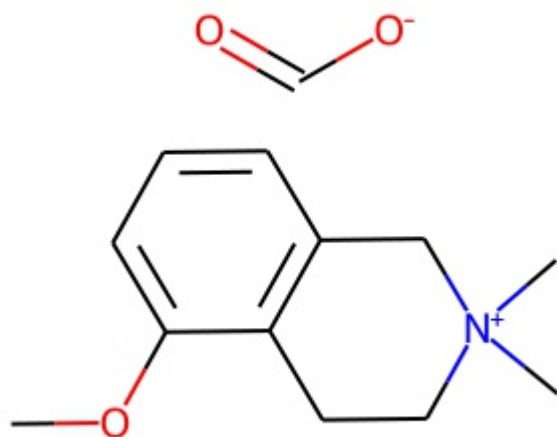p_risky at threshold of 5: [0.374]

interesting mol: COc1cccc2c1CC(C[N+](C)(C)C)CC2.O=C[O-]
predicted mean: [5.894]
predicted standard deviation: [0.522]
95% CI: [4.849] - [6.939]
aleatoric uncertainty: [0.477]
epistemic uncertainty: [0.22]
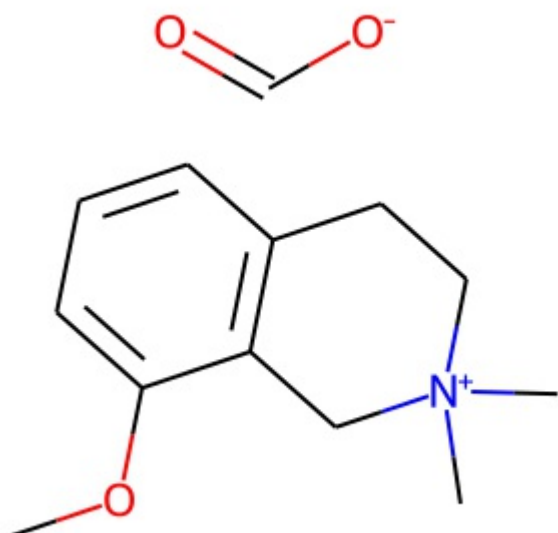p_risky at threshold of 5: [0.036]

interesting mol: COc1cccc2c1CCC(C[N+](C)(C)C)C2.O=C[O-]
predicted mean: [6.01]
predicted standard deviation: [0.521]
95% CI: [4.967] - [7.052]
aleatoric uncertainty: [0.476]
epistemic uncertainty: [0.237]
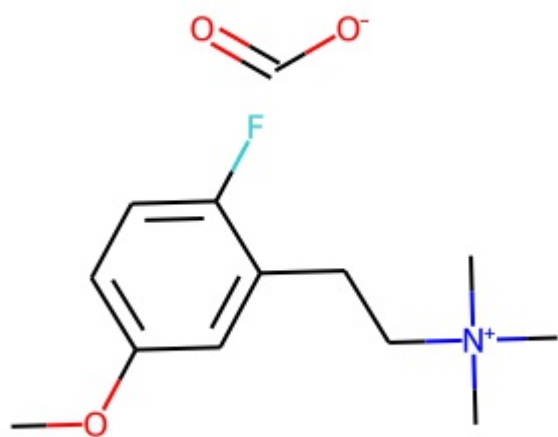p_risky at threshold of 5: [0.034]

interesting mol: COc1cccc(C(O)C[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.512]
predicted standard deviation: [0.522]
95% CI: [4.467] - [6.557]
aleatoric uncertainty: [0.491]
epistemic uncertainty: [0.2]
p_risky at threshold of 5: [0.158]
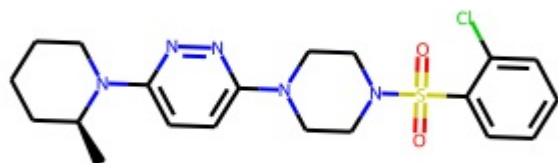

interesting mol: COc1cccc2c1CC[N+](C)(C)C2.O=C[O-]
predicted mean: [5.704]
predicted standard deviation: [0.541]
95% CI: [4.622] - [6.786]
aleatoric uncertainty: [0.485]
epistemic uncertainty: [0.207]
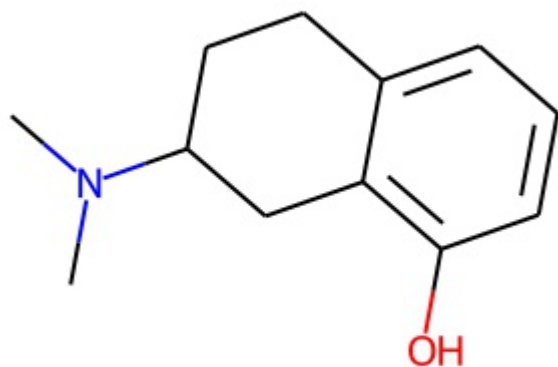p_risky at threshold of 5: [0.108]

interesting mol: COc1cccc2c1C[N+](C)(C)CC2.O=C[O-]
predicted mean: [5.754]
predicted standard deviation: [0.506]
95% CI: [4.742] - [6.765]
aleatoric uncertainty: [0.484]
epistemic uncertainty: [0.214]
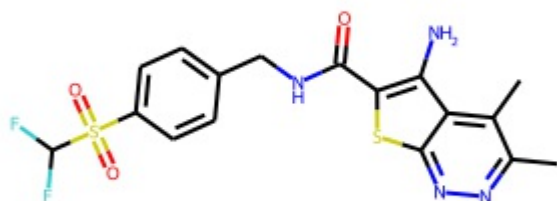p_risky at threshold of 5: [0.089]

interesting mol: COc1ccc(F)c(CC[N+](C)(C)C)c1.O=C[O-]
predicted mean: [5.282]
predicted standard deviation: [0.551]
95% CI: [4.179] - [6.385]
aleatoric uncertainty: [0.5]
epistemic uncertainty: [0.255]
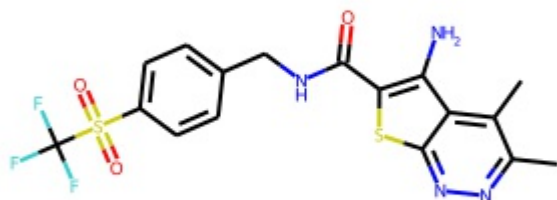p_risky at threshold of 5: [0.33]

interesting mol: C[C@H]1CCCCN1c1ccc(N2CCN(S(=O)(=O)c3ccccc3Cl)CC2)nn1
predicted mean: [7.407]
predicted standard deviation: [0.532]
95% CI: [6.344] - [8.47]
aleatoric uncertainty: [0.424]
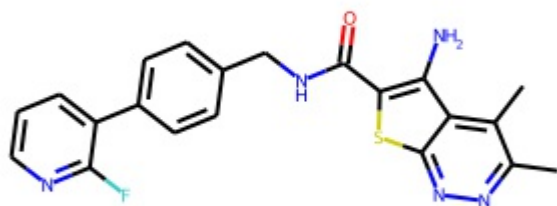epistemic uncertainty: [0.26]
p_risky at threshold of 5: [0.]

interesting mol: CN(C)C1CCc2cccc(O)c2C1
predicted mean: [5.943]
predicted standard deviation: [0.51]
95% CI: [4.923] - [6.963]
aleatoric uncertainty: [0.478]
epistemic uncertainty: [0.195]
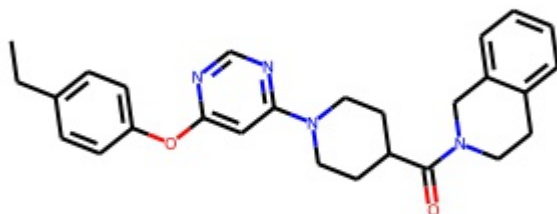p_risky at threshold of 5: [0.046]

interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(S(=O)(=O)C(F)F)cc3)c(N)c2c1C
predicted mean: [6.981]
predicted standard deviation: [0.546]
95% CI: [5.889] - [8.073]
aleatoric uncertainty: [0.437]
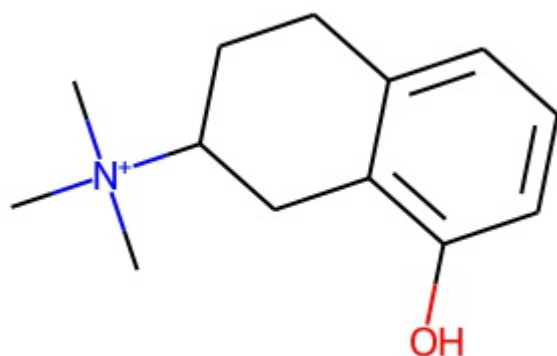epistemic uncertainty: [0.277]
p_risky at threshold of 5: [0.]

interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(S(=O)(=O)C(F)(F)F)cc3)c(N)c2c1C
predicted mean: [6.379]
predicted standard deviation: [0.525]
95% CI: [5.329] - [7.429]
aleatoric uncertainty: [0.455]
epistemic uncertainty: [0.276]
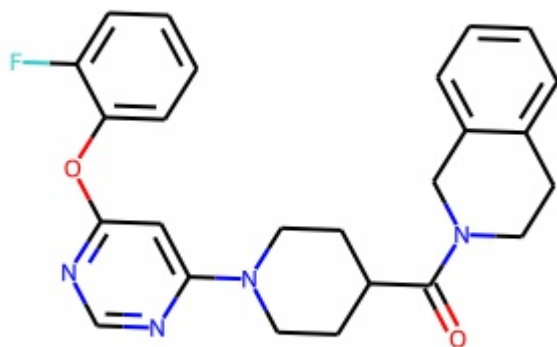p_risky at threshold of 5: [0.004]

interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(-c4cccnc4F)cc3)c(N)c2c1C
predicted mean: [5.588]
predicted standard deviation: [0.538]
95% CI: [4.513] - [6.664]
aleatoric uncertainty: [0.489]
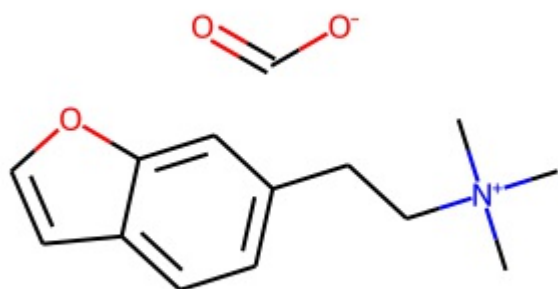epistemic uncertainty: [0.24]
p_risky at threshold of 5: [0.142]

interesting mol: CCc1ccc(Oc2cc(N3CCC(C(=O)N4CCc5ccccc5C4)CC3)ncn2)cc1
predicted mean: [4.731]
predicted standard deviation: [0.555]
95% CI: [3.621] - [5.842]
aleatoric uncertainty: [0.52]
epistemic uncertainty: [0.22]
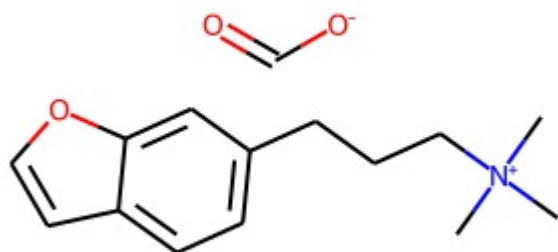p_risky at threshold of 5: [0.712]

interesting mol: C[N+](C)(C)C1CCc2cccc(O)c2C1
predicted mean: [6.367]
predicted standard deviation: [0.509]
95% CI: [5.35] - [7.384]
aleatoric uncertainty: [0.461]
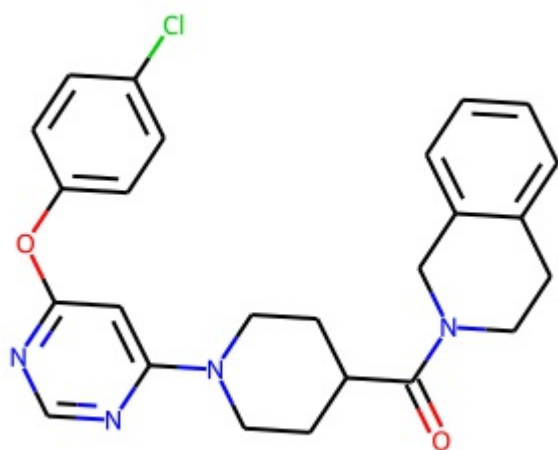epistemic uncertainty: [0.181]
p_risky at threshold of 5: [0.003]

interesting mol: O=C(C1CCN(c2cc(Oc3ccccc3F)ncn2)CC1)N1CCc2ccccc2C1
predicted mean: [5.636]
predicted standard deviation: [0.546]
95% CI: [4.545] - [6.727]
aleatoric uncertainty: [0.486]
epistemic uncertainty: [0.244]
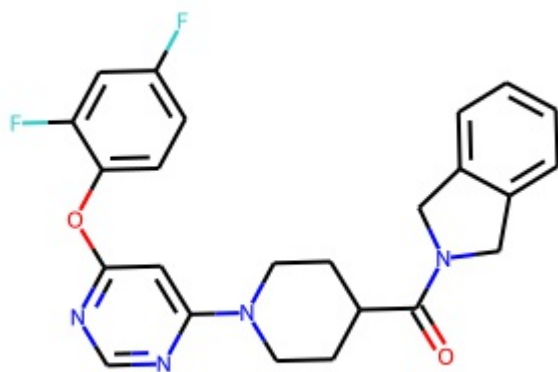p_risky at threshold of 5: [0.102]

interesting mol: C[N+](C)(C)CCc1ccc2ccoc2c1.O=C[O-]
predicted mean: [4.663]
predicted standard deviation: [0.595]
95% CI: [3.472] - [5.854]
aleatoric uncertainty: [0.521]
epistemic uncertainty: [0.242]
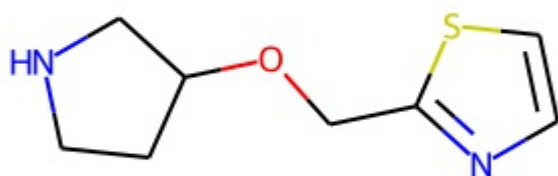p_risky at threshold of 5: [0.728]

interesting mol: C[N+](C)(C)CCCc1ccc2ccoc2c1.O=C[O-]
predicted mean: [5.019]
predicted standard deviation: [0.535]
95% CI: [3.948] - [6.089]
aleatoric uncertainty: [0.509]
epistemic uncertainty: [0.218]
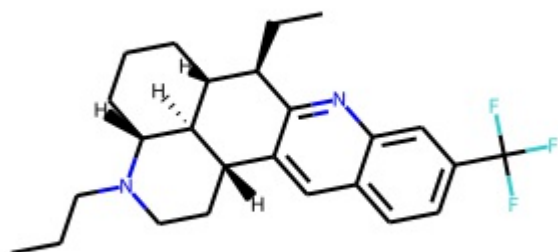p_risky at threshold of 5: [0.511]

interesting mol: O=C(C1CCN(c2cc(Oc3ccc(Cl)cc3)ncn2)CC1)N1CCc2ccccc2C1
predicted mean: [5.192]
predicted standard deviation: [0.554]
95% CI: [4.083] - [6.3]
aleatoric uncertainty: [0.503]
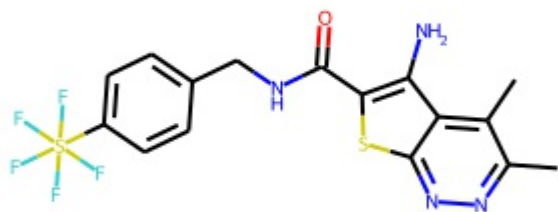epistemic uncertainty: [0.243]
p_risky at threshold of 5: [0.377]

interesting mol: O=C(C1CCN(c2cc(Oc3ccc(F)cc3F)ncn2)CC1)N1Cc2ccccc2C1
predicted mean: [5.834]
predicted standard deviation: [0.499]
95% CI: [4.836] - [6.832]
aleatoric uncertainty: [0.479]
epistemic uncertainty: [0.225]
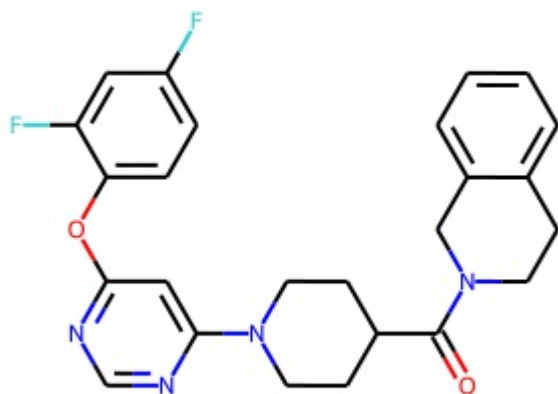p_risky at threshold of 5: [0.053]

interesting mol: c1csc(COC2CCNC2)n1
predicted mean: [6.455]
predicted standard deviation: [0.533]
95% CI: [5.388] - [7.522]
aleatoric uncertainty: [0.453]
epistemic uncertainty: [0.259]
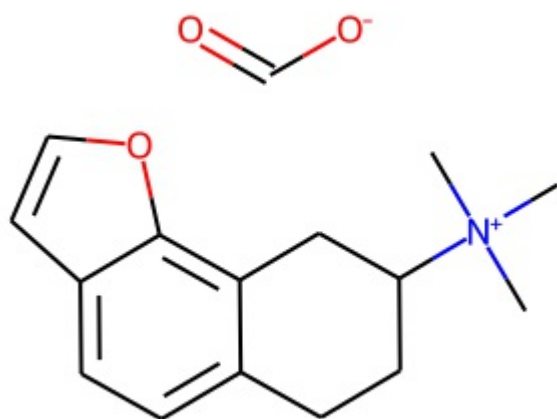p_risky at threshold of 5: [0.002]

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: [5.063]
predicted standard deviation: [0.521]
95% CI: [4.022] - [6.105]
aleatoric uncertainty: [0.507]
epistemic uncertainty: [0.254]
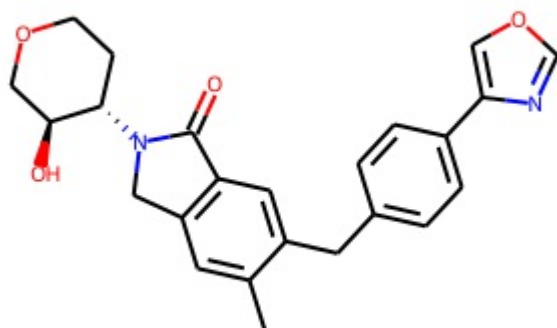p_risky at threshold of 5: [0.486]

interesting mol: Cc1nnc2sc(C(=O)NCc3ccc(S(F)(F)(F)(F)F)cc3)c(N)c2c1C
predicted mean: [5.291]
predicted standard deviation: [0.571]
95% CI: [4.148] - [6.433]
aleatoric uncertainty: [0.497]
epistemic uncertainty: [0.253]
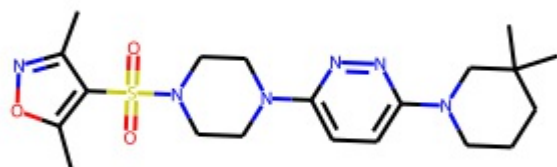p_risky at threshold of 5: [0.278]

interesting mol: O=C(C1CCN(c2cc(Oc3ccc(F)cc3F)ncn2)CC1)N1CCc2ccccc2C1
predicted mean: [5.806]
predicted standard deviation: [0.537]
95% CI: [4.732] - [6.879]
aleatoric uncertainty: [0.479]
epistemic uncertainty: [0.241]
p_risky at threshold of 5: [0.061]

interesting mol: C[N+](C)(C)C1CCc2ccc3ccoc3c2C1.O=C[O-]
predicted mean: [5.828]
predicted standard deviation: [0.519]
95% CI: [4.79] - [6.867]
aleatoric uncertainty: [0.479]
epistemic uncertainty: [0.208]
p_risky at threshold of 5: [0.055]

interesting mol: Cc1cc2c(cc1Cc1ccc(-c3cocn3)cc1)C(=O)N([C@H]1CCOC[C@@H]1O)C2
predicted mean: [5.923]
predicted standard deviation: [0.555]
95% CI: [4.813] - [7.032]
aleatoric uncertainty: [0.476]
epistemic uncertainty: [0.271]
p_risky at threshold of 5: [0.046]

interesting mol: Cc1noc(C)c1S(=O)(=O)N1CCN(c2ccc(N3CCCC(C)(C)C3)nn2)CC1
predicted mean: [5.881]
predicted standard deviation: [0.58]
95% CI: [4.721] - [7.04]
aleatoric uncertainty: [0.475]
epistemic uncertainty: [0.276]
p_risky at threshold of 5: [0.067]

In [28]: