

| SMILES  | Name   | PubChem_CID | SIDER_CID | Source  | logBB | Class | Class_Verbose | MW  | TPSA | XLogP | NHD | NHA | NRB | Synonyms     | Side_Effects | Indications |
|---|--|-------------|-----------|---|-------|-------|---------------|-----|------|-------|-----|-----|-----|--------------|--------------|-------------|
| CN1CCC2=C   | (+)-Bicuculline  | 10237       | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -     | 0     | Does not Pass | 367 | 66.5 | 2.6   | 0   | 7   | 1   | ["(+)-Bicuc  | -            | -           |
| CCC[C@@H]   | (+)-Secobarbital   | 31143       | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | 0.2   | 1     | Passes        | 238 | 75.3 | 2     | 2   | 3   | 5   | ["(+)-Secol  | -            | -           |
| CNCCC(Oc  | (+)-Duloxetine   | 122252      | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -     | 1     | Passes        | 297 | 49.5 | 4.3   | 1   | 3   | 6   | ["(+)-Dulo   | -            | -           |
| C   | (11c)methane   | 297         | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -     | 1     | Passes        | 16  | 0    | 0.6   | 0   | 0   | 0   | ["(11c)met   | -            | -           |
| c1ccccc1C   | (2S,3S)-2-(Diphenylmethyl)-2-methylpropane-1-thiol                                     | 9931510     | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | 0.37  | 1     | Passes        | 413 | 24.5 | 5.4   | 1   | 3   | 7   | ["(2S,3S)-2  | -            | -           |
| CC5(C)SC4   | (2S,5R,6R)-6-(3-Amino-2-methoxyphenyl)-5,6-dihydro-2H-pyran-2-one                      | 20056959    | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -     | 0     | Does not Pass | 394 | 138  | -0.9  | 3   | 6   | 3   | ["(2S,5R,6R  | -            | -           |
| CC1OC1P(=O)(O)C   | (3-Methyloxiran-2-ylidene)phosphine oxide  | 3417        | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -     | 1     | Passes        | 138 | 70.1 | -1.4  | 2   | 4   | 1   | ["(3-Methy   | -            | -           |
| OCC(=O)[C@H]1CC[C@@H]2[C@@H](C(=O)O)[C@@H](C(=O)O)[C@H]12 | (8S,9S,10R,13S,14S,15S)-8,9,10-trihydroxy-13,14,15-trimethyl-8-azabicyclo[3.3.1]nonane | 11245343    | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -0.18 | 1     | Passes        | 360 | 94.8 | 1.6   | 3   | 5   | 2   | ["(8S,9S,10  | -            | -           |
| CC(C)(C)C(=O)N  | (R)-Stiripentol  | 39524       | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | -     | 1     | Passes        | 234 | 38.7 | 3.6   | 1   | 3   | 3   | ["(R)-Stirip | -            | -           |
| CN[C@H](C)C   | (R)-propylhexedrine  | 111165      | -         | <a href="https://doi.org/10.26434/chemrxiv-2020-08-01">https://doi.org/10.26434/chemrxiv-2020-08-01</a> | 1.08  | 1     | Passes        | 155 | 12   | 3.5   | 1   | 1   | 3   | ["(R)-propy  | -            | -           |