Compound Name CASRN SMILES MW JRC Rat Clint Fub logP
pKa
"2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane (HPTE)" 2971-36-0
C(C(C1C=CC(=CC=1)O)C2C=CC(=CC=2)O)(Cl)(Cl)Cl 317.5949
56.8622 0.005 4.55 7.282
Abamectin 71751-41-2
CO[C@H]1C[C@@H](O[C@@H](C)[C@@H]1O)O[C@@H]2[C@@H](OC)C[C@@H](O[C@H]2
C)O[C@@H]3C(\C)=C\C[C@@H]7C[C@H](OC(=O)[C@@H]4/C=C(/C)[C@@H](O)[C@H]5OC/C(=C\C=
C\[C@@H]3C)[C@@]45O)C[C@]6(/C=C\[C@H](C)[C@H](O6)[C@@H](C)CC)O7 873.0769
3.6216 0.0669 4.39 11.144
Acetaminophen 103-90-2 C1(=CC=C(C=C1)O)NC(C)=O 151.1626 Y
0.260944444 0.79 0.46 9.51
Amitraz 33089-61-1 Cc2cc(C)ccc2/N=C/N(C)/C=N/c1ccc(C)cc1C 293.406
19.30184 0.005 5.5 0.175
Anilazine 101-05-3 ClC1=NC(=NC(=N1)NC2=CC=CC=C2Cl)Cl 275.5218
22.49708 0.005 3.88 -0.428
Atrazine 1912-24-9 ClC1=NC(=NC(=N1)NC(C)C)NCC 215.6833 Y Y
6.209374649 0.123704301 2.61 0.789
Azinphos-methyl 86-50-0 O=C1C2=C(C=CC=C2)N=NN1CSP(=S)(OC)OC
317.3243 12.29811 0.213679 2.75 -0.424
Azoxystrobin 131860-33-8
N#CC1=CC=CC=C1OC2=NC=NC(OC3=CC=CC=C3/C(C(OC)=O)=C\OC)=C2 403.3875
14.2876 0.047634 2.5 0.612
Bendiocarb 22781-23-3 O=C(NC)OC1=CC=CC2=C1OC(C)(C)O2 223.2252
10.0244 0.197104 1.7 11.902
Benomyl 17804-35-2 CCCCNC(=O)n1c2ccccc2nc1NC(=O)OC 290.3177
72.2852 0.005 2.12 2.635
Bensulide 741-58-2 S(=O)(=O)(C1=CC=CC=C1)NCCSP(=S)(OC(C)C)OC(C)C
397.5134 87.05810055 0.006078373 4.2 10.795
Bifenazate 149877-41-8 O=C(NNC1=C(OC)C=CC(C2=CC=CC=C2)=C1)OC(C)C
300.3523 5.6355 0.836 4.14 0.641
Bisphenol-A 80-05-7 C(C1C=CC(=CC=1)O)(C2=CC=C(C=C2)O)(C)C 228.2863
Y 25.03752924 0.06821704 3.32 7.889
Bromoxynil 1689-84-5 C1=C(Br)C(O)=C(Br)C=C1C#N 276.9128
4.2829 0.5 3.39 5.26
Buprofezin 69327-76-0 O=C1N(C(C)C)/C(SCN1C2=CC=CC=C2)=N/C(C)(C)C 305.4383
11.59718193 0.005 4.3 0.633
Butralin 33629-47-9 [O-][N+](C1=CC(C(C)(C)C)=CC([N+]([O-])=O)=C1NC(C)CC)=O
295.3342 13.7939 0.005 4.93 12.253
Clorophene 120-32-1 OC1=C(C=C(C=C1)Cl)CC2=CC=CC=C2 218.6788
12.9387 0.005 4.18 9.359
Cyclanilide 113136-77-9 O=C(NC2=CC=C(Cl)C=C2Cl)C1(C(O)=O)CC1 274.1001
0.5336 0.984015 1.84 3.984
Cyproconazole 94361-06-5 ClC1=CC=C(C(CN2C=NC=N2)(C(C)C3CC3)O)C=C1 291.7759
Y Y 1.5875 0.108556 2.9 -2.152
Cyprodinil 121552-61-2 CC1=NC(NC3=CC=CC=C3)=NC(C2CC2)=C1 225.289
0.838878676 0.005 4 4.914
Dazomet 533-74-4 CN1CN(C)CSC1=S 162.2763 12.41844
0.891427 1.4 4.285
Dichloran 99-30-9 O=[N+](C1=CC(=C(C(=C1)Cl)N)Cl)[O-] 207.0142
3.312946 0.005 2.8 -1.53
Dicofol 115-32-2 OC(C1=CC=C(C=C1)Cl)(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl 370.4857
2.9512 0.005 5.02 9.666
Diniconazole 83657-24-3 OC(C(C)(C)C)/C(N2N=CN=C2)=C\C1=C(Cl)C=C(Cl)C=C1
326.221 0 0.019468 4.3 -2.837
Etoxazole 153233-91-1 FC2=C(C(F)=CC=C2)C1=NC(C3=C(OCC)C=C(C(C)(C)C)C=C3)CO1

359.4096 15.42613225 0.005 7.21 5.011
Fenarimol 60168-88-9 OC(C2=CN=CN=C2)(C3=CC=C(Cl)C=C3)C1=CC=CC=C1Cl
331.196 0.0288 0.03671 3.6 1.5
Fenoxycarb 72490-01-8 O=C(NCCOC1=CC=C(OC2=CC=CC=C2)C=C1)OCC 301.3371
4.424073126 0.005 4.3 11.441
Fluazinam 79622-59-6 ClC1=C(NC2=C([N+]([O-])=O)C(Cl)=C(C(F)(F)F)C=C2[N+]([O-
])=O)N=CC(C(F)(F)F)=C1 465.0917 24.7601 0.005 3.56 1.659
Fludioxonil 131341-86-1 FC3(F)OC(C(O3)=CC=C2)=C2C1=CNC=C1C#N 248.185
37.0472 0.005 4.12 11.734
Fluoxastrobin 361377-29-9
ClC1=C(OC2=NC=NC(OC3=C(\C(C4=NOCCO4)=N/OC)C=CC=C3)=C2F)C=CC=C1
458.8269 0 0.036201 2 -1.24
Fluroxypyr-meptyl 81406-37-3 FC1=C(Cl)C(N)=C(Cl)C(OCC(OC(C)CCCCCC)=O)=N1
367.2432 138.110265 0.005 4.53 0.383
Flusilazole 85509-19-9 C[Si](Cn1cncn1)(c2ccc(F)cc2)c3ccc(F)cc3 315.3927 Y
Y 5.17 0.028931 3.7 2.5
Hexaconazole 79983-71-4 ClC1=CC(Cl)=CC=C1C(CCCC)(O)CN2C=NC=N2 314.2103
Y Y 3.7375 0.041 3.9 -2.155
Hexythiazox 78587-05-0 C[C@H]2[C@@H](SC(=O)N2C(=O)NC1CCCCC1)c3ccc(Cl)cc3
352.8788 9.5213 0.005 5.57 2.443
HPTE 2971-36-0 C(C(C1C=CC(=CC=1)O)C2C=CC(=CC=2)O)(Cl)(Cl)Cl 317.5949
56.8622 0.005 4.55 7.282
Imazalil 35554-44-0 Clc2ccc(C(OCC=C)Cn1ccnc1)c(Cl)c2 297.1798 Y Y
0 0.029558 3.82 7.203
Myclobutanil 88671-89-0 Clc1ccc(cc1)C(CCCC)(Cn2cncn2)C#N 288.7753 Y Y
16.3986 0.084287 2.94 -2.208
Niclosamide 50-65-7 O=C(NC2=CC=C([N+]([O-])=O)C=C2Cl)C1=C(O)C=CC(Cl)=C1
327.1196 12 0.005 4.56 6.372
Norflurazon 27314-13-2 FC(F)(F)c1cc(ccc1)N2\N=C/C(NC)=C(/Cl)C2=O 303.6676
0 0.184057 2.3 0.232
Oryzalin 19044-88-3 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)S(N)(=O)=O
346.3595 13.512 0.005 3.73 9.357
Oxadiazon 19666-30-9 O=C2O\C(=N/N2c1cc(OC(C)C)c(Cl)cc1Cl)C(C)(C)C 345.221
4.3745 0.005 4.8 -2.225
Oxamyl 23135-22-0 O=C(C(=NOC(=O)NC)SC)N(C)C 219.2614
0 0.792577 -0.47 9.681
Oxytetracycline dihydrate 6153-64-6
O=C1[C@](C(O)=C2[C@@]3([H])[C@@](O)(C)C4=C(C(O)=CC=C4)C2=O)(O)[C@]([C@H]3O)([
H])[C@H](N(C)C)C(O)=C1C(N)=O.O.O 496.4645 0 0.398168608 -0.9
3.346
Paclobutrazol 76738-62-0 O[C@H]([C@H](Cc1ccc(Cl)cc1)n2cncn2)C(C)(C)C 293.7918
6.2058 0.153767 3.2 -2.128
Perfluorooctanoic acid (PFOA) 335-67-1
O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F 414.0684 Y Y
4.5493 0.005 6.3 -1.032
Permethrin 52645-53-1 C1=CC=C(OC2=CC=CC=C2)C=C1COC(=O)C3C(C)(C)C3C=C(Cl)Cl
391.2877 Y Y 22.5867 0.005 6.5 3.95
Phosalone 2310-17-0 CCOP(=S)(OCC)SCN1c2ccc(Cl)cc2OC1=O 367.8086
34.4366 0.005 4.38 -1.3
Prochloraz 67747-09-5 O=C(N(CCOc1c(Cl)cc(Cl)cc1Cl)CCC)n2ccnc2 376.6654
3.9782 0.02237 4.1 5.504
Prodiamine 29091-21-2 NC1=C(C(F)(F)F)C=C([N+]([O-])=O)C(N(CCC)CCC)=C1[N+]([O-])=O
350.2937 7.2155 0.005 4.1 11.074
Propanil 709-98-8 C1=C(Cl)C(Cl)=CC=C1NC(=O)CC 218.0799
38.8981 0.005 3.07 -2.26
Pyraclostrobin 175013-18-0 ClC3=CC=C(C=C3)N(C=C2)N=C2OCC1=C(C=CC=C1)N(C(OC)=O)OC

387.8169 53.93250871 0.005 5.45 -1.841
Pyridaben 96489-71-3 O=C1N(C(C)(C)C)N=CC(SCC2=CC=C(C(C)(C)C)C=C2)=C1Cl
364.9326 14.4079 0.005 6.37 -1.442
Pyrimethanil 53112-28-0 CC1=NC(NC2=CC=CC=C2)=NC(C)=C1 199.2517
8.922 0.016733 2.84 4.856
Pyriproxyfen 95737-68-1 CC(OC3=NC=CC=C3)COC2=CC=C(C=C2)OC1=CC=CC=C1
321.3698 17.7465 0.005 5.55 3.066
Simazine 122-34-9 ClC1=NC(=NC(=N1)NCC)NCC 201.6567 Y
6.32606 0.284499 2.18 0.789
Spiroxamine 118134-30-8 CC(C)(C)C(CC2)CCC12OC(CO1)CN(CCC)CC 297.476
0 0.005446 5.51 8.367
Tebufenpyrad 119168-77-3 O=C(NCC2=CC=C(C(C)(C)C)C=C2)C1=C(Cl)C(CC)=NN1C
333.8557 15.936 0.005 4.61 -2.162
Tebupirimfos 96182-53-5 S=P(OCC)(OC1=CN=C(C(C)(C)C)N=C1)OC(C)C 318.3721
15.7151 0.005 4.19 1.776
Tetraconazole 112281-77-3 ClC2=C(C=CC(Cl)=C2)C(COC(F)(F)C(F)F)CN1N=CN=C1
372.1456 0 0.024838 3.56 -2.166
Thidiazuron 51707-55-2 O=C(NC2=CC=CC=C2)NC1=CN=NS1 220.251
4.9203 0.028375 1.77 2.388
Thiophanate-methyl 23564-05-8 S=C(Nc1ccccc1NC(=S)NC(=O)OC)NC(=O)OC 342.394
3.4575 0.427007 1.4 -2.621
Triadimefon 43121-43-3 CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n2cncn2 293.7487 Y
Y 18.02415303 0.114217227 2.77 -2.289
Triadimenol 55219-65-3 OC(C(C)(C)C)C(N2N=CN=C2)OC1=CC=C(Cl)C=C1 295.7646
0 0.125809 2.9 -2.188
Triclosan 3380-34-5 Clc2cc(Cl)ccc2Oc1ccc(Cl)cc1O 289.5418 Y Y
48.76860004 0.005 4.76 6.847
Triflumizole 68694-11-1 ClC2=CC(C(F)(F)F)=C(C=C2)/N=C(COCCC)/N1C=NC=C1
345.7473 8.669 0.005 1.4 2.666
Triticonazole 131983-72-7 OC1(CN3N=CN=C3)C(C)(C)CC\C1=C/C2=CC=C(Cl)C=C2
317.8132 Y Y 6.1175 0.137257 3.29 -2.108
Zoxamide 156052-68-5 O=C(NC(CC)(C)C(CCl)=O)C1=CC(Cl)=C(C)C(Cl)=C1 336.6413
53.46463746 0.010310358 4.35 11.547