

These PNECs are published on a forum to facilitate collaboration between participating organizations. This list includes published PNECs data and those provided by pharmaceutical companies, and were not calculated by the WET Center.

These predicted no-effect concentrations, PNECs, are provided to facilitate environmental risk assessment of pharmaceuticals in surface water downstream of the mixing zone (i.e., not at the point of discharge or entry into the environment) by interested stakeholders. The chronic PNECs were derived from guideline studies (e.g., OECD, USFDA, USEPA) and the application of an appropriate assessment factor. This is the same data required to register a new pharmaceutical in Europe. For some pharmaceuticals, only acute data are available and were used with the appropriate assessment factor. The references are to peer reviewed publications, and also to unpublished internal company documents for a limited number of compounds.

Compound Name	log Kow	PNEC Calculated from Acute Data (µg/L)	PNEC Calculated from Chronic Data (µg/L)	Reference		
5-fluorouracil	-0.89		0.2	Vestel et al. 2016		
abiraterone acetate	5.12		0.0013	Vestel et al. 2016		
acyclovir	-1.2		200	Vestel et al. 2016		
AIC (5-amino-1H-imidazole-4-carboxamide)	-1		82.4	Vestel et al. 2016		
alfuzosin	1.51		200	Vestel et al. 2016		
alvimopan	0.52		3.4	Vestel et al. 2016		
anastrozole	1.58		1	Vestel et al. 2016		
anidulafungin	5.09		5	Vestel et al. 2016		
aprepitant	4.75		1.8	Vestel et al. 2016		
aripiprazole	2.95		0.261	Vestel et al. 2016		
articaine		92		Johnson & Johnson		
atazanavir	3.3		410	Vestel et al. 2016		
atenolol	0.015		148	Vestel et al. 2016		
atorvastatin	1.42		14	Vestel et al. 2016		
azithromycin	0.48		0.019	Vestel et al. 2016		
bambuterol HCl		71		Murray-Smith et al. 2011		
bedaquiline	2.93		0.077	Vestel et al. 2016		
bezafibrate	4.25		1000	Vestel et al. 2016		

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bicalutamide	2.54		1	Vestel et al. 2016		
budesonide	3.3	8.6		Murray-Smith et al. 2011		
bupivacaine HCl monohydrate		39		Murray-Smith et al. 2011		
bupropion	1.54		10	Vestel et al. 2016		
canagliflozine	3.42		56	Vestel et al. 2016		
candesartan	1.63		100	Vestel et al. 2016		
capecitabine	4.5		280	Vestel et al. 2016		
carisbamate	1.2		96	Vestel et al. 2016		
carvedilol	2.73		5	Vestel et al. 2016		
casopitant	4.13		63.9	Vestel et al. 2016		
ceftobiprole	-2.2		0.022	Vestel et al. 2016		
celecoxib	3.18		1.1	Vestel et al. 2016		
cetirizine		100		Johnson & Johnson		
chlorthalidone		80		Snape 2015		
cimetidine	0.199		176	Vestel et al. 2016		
cinacalcet hydrochloride	4.79		0.25	Vestel et al. 2016		
cisapride		1000		Johnson & Johnson		
clomethiazole edisilate		62		Murray-Smith et al. 2011		
clopidogrel bisulfate	3.96		31	Vestel et al. 2016		
codeine			216 or 500	Vestel et al. 2016 or J&J		
dalcetrapib	6		0.0074	Vestel et al. 2016		

Compound Name	log Kow	PNEC Calculated from Acute Data (µg/L)	PNEC Calculated from Chronic Data (µg/L)	Reference		
dapagliflozin			100	Snape 2015		
dapoxetine HCl	5.09		0.73	Vestel et al. 2016		
darunavir	2.47		940	Vestel et al. 2016		
diazepam	2.99		27.3	Vestel et al. 2016		
diclofenac	4.51		32	Vestel et al. 2016		
diphenhydramine			0.1	Johnson & Johnson		
domperidone	3.96	12		Johnson & Johnson		
doripenem	-2.7		0.11	Vestel et al. 2016		
doxorubicin		1.8		Johnson & Johnson		
dronedarone	4.63		0.4	Vestel et al. 2016		
efavirenz	5.4		2.6	Vestel et al. 2016		
entecavir	-0.82		32	Vestel et al. 2016		
eplerenone	1.02		20	Vestel et al. 2016		
eplivanserin	2.29		11.9	Vestel et al. 2016		
erlotinib HCl	3.57		52	Vestel et al. 2016		
esomeprazole Na	2.24		100	Vestel et al. 2016		
estradiol	4.01		0.002	Caldwell et a. 2012		
estriol			0.06	Caldwell et al. 2012		
estrone			0.006	Caldwell et al. 2012		
ethinylestradiol	3.67		0.0001	Caldwell et al. 2012		
etoricoxib	2.3		75	Vestel et al. 2016		

Compound Name	log Kow	PNEC Calculated from Acute Data (µg/L)	PNEC Calculated from Chronic Data (µg/L)	Reference		
ezetimibe	4.36		5.1	Vestel et al. 2016		
felodipine	5	0.005		Murray-Smith et al. 2011		
formoterol fumarate	0.41	94		Murray-Smith et al. 2011		
fosamprenavir Ca	1		2000	Vestel et al. 2016		
fulvestrant	7.67		0.0001	Vestel et al. 2016		
gefitinib	4.15		3.2	Vestel et al. 2016		
haloperidol	4.3		0.4	Johnson & Johnson		
hydrochlorothiazide	0.04		200	Vestel et al. 2016		
ibuprofen			1	Johnson & Johnson		
ibrutinib	4		2	Vestel et al. 2016		
irbesartan			704	Vestel et al. 2016		
ketoconazole	3.78		0.05	Vestel et al. 2016		
lamotrigine	1.4		150	Vestel et al. 2016		
laropiprant	2.4		950	Vestel et al. 2016		
lidocaine hydrochloride	1.6	110		Murray-Smith et al. 2011		
linezolid	0.55		20	Vestel et al. 2016		
lisinopril dihydrate	-1.01	100		Murray-Smith et al. 2011		
mepivacaine HCl		59		Murray-Smith et al. 2011		
meropenem		1.5		Snape 2015		
metformin	-2		1030	Vestel et al. 2016		
methylphenidate HCl	-3.06		77	Vestel et al. 2016		

Compound Name	log Kow	PNEC Calculated from Acute Data (µg/L)	PNEC Calculated from Chronic Data (µg/L)	Reference		
metoprolol succinate	-0.9	7.3		Murray-Smith et al. 2011		
miconazole nitrate	3.4		0.2	Vestel et al. 2016		
montelukast	4.3		7.3	Vestel et al. 2016		
naproxen			4.2	Murray-Smith et al. 2011		
omeprazole	2.24	83		Snape 2015		
paliperidone	2.39		250	Vestel et al. 2016		
pazopanib	3.33		15	Vestel et al. 2016		
pregabalin	-1.9		100	Vestel et al. 2016		
prilocaine HCl	1.4	61		Murray-Smith et al. 2011		
propofol	3.9	0.37		Vestel et al. 2016		
propranolol HCl	0.72		0.02	Vestel et al. 2016		
quetiapine fumarate			10 (8)	Vestel et al. 2016 (Murray-Smith)		
raltegravir	0.328		860	Vestel et al. 2016		
ramipril		100		Murray-Smith et al. 2011		
ribavirin	-2.29		0.097	Vestel et al. 2016		
ridaforolimus	4.68		0.0031	Vestel et al. 2016		
rilpivirine	4.66		2	Vestel et al. 2016		
rimonabant	5.61		1.6	Vestel et al. 2016		
rivaroxaban			8.6	Vestel et al. 2016		
ropivacaine HCl		34		Murray-Smith et al. 2011		
rosuvastatin calcium	0.28		1.8	Vestel et al. 2016		

Compound Name	log Kow	PNEC Calculated from Acute Data (µg/L)	PNEC Calculated from Chronic Data (µg/L)	Reference		
saxagliptin	0.114		190	Vestel et al. 2016		
simeprevir			0.1	Vestel et al. 2016		
sitagliptin	-0.03		390	Vestel et al. 2016		
sulfamethoxazole	0.89		0.2	Vestel et al. 2016		
sutent	2.4		2.7	Vestel et al. 2016		
tamoxifen citrate	3.68		0.49	Vestel et al. 2016		
tapentadol	2.87		53	Vestel et al. 2016		
taranabant	5.49		2.1	Vestel et al. 2016		
telcagepant	3.65		350	Vestel et al. 2016		
terbutaline sulphate	-1.8	240		Murray-Smith et al. 2011		
ticagrelor	4.02		53	Vestel et al. 2016		
topiramate	3.74	93		Vestel et al. 2016		
tramadol		73		Vestel et al. 2016		
trimethoprim	0.91		120	Vestel et al. 2016		
vicriviroc maleate	0.04		270	Vestel et al. 2016		
vorinostat	1.42		1.1	Vestel et al. 2016		
zafirlukast	2.3		12.8	Vestel et al. 2016		
zolmitriptan			100	Vestel et al. 2016		