Drug Database

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The calculated values (DrugBank/Chrmaxon Marvin) are reliable to roughly ±0.5 pKa units.

NRTIs (Nucleoside/Nucleotide Reverse Transcriptase Inhibitors)

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
TFV	Tenofovir (active drug)	-1.6	3.8, 6.7	Phosphonate -OH (×2)	Experimental (DrugBank) & Zhang T. et al. 2012. Eur J Pharm Biopharm.
TDF	Tenofovir Disoproxil Fumarate	1.25	3.75	Phosphonate -OH (×2)	FDA label & Watkins M.E., et al. 2017. J Pharm Sci.
TAF	Tenofovir Alafenamide	1.6	3.96	Adenine amino / phosphoramidate system (overall molecular ionization)	Product Monograph (Gilead Sciences)
FTC	Emtricitabine	-0.43	2.65	Cytosine N3	National Library of Medicine
3TC	Lamivudine	-1.4	4.3	Cytosine N3 (basic)	Strauch S., et al. 2011. J Pharm Sci.
AZT	Zidovudine	0.05	9.8	Thymine N3 (acid)	Soares K.C.C., et al. 2013. J Pharm Sci.
ABC	Abacavir (in form of Abacavir Sulfate)	1.20	5.06	Purine N (basic)	Apotex Product Monograph, 2017, National Library of Medicine

NRTTI (Nucleoside/Nucleotide Reverse Transcriptase Translocation Inhibitor)

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
ISL	Islatravir	-0.42	0.79	purine N	Drugbank Chemaxon

NNRTI (Non-Nucleoside Reverse Transcriptase Inhibitor)

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
EFV	Efavirenz	4.6	10.2	Cyclic carbamate	Adeola et.al. Elsevier
NVP	Nevirapine	2.5	2.8	Pyridine N and Amide N	Adeola et.al. Elsevier
RPV	Rilpivirine	4.86	5.6	Aminopyrimidine group	Usach, et al. J Int AIDS Soc. 16(1): 18567. (2013)
ETR	Etravirine	5.2	3.5	primary amine group (-NH_2)	Usach, et al. J Int AIDS Soc. 16(1): 18567. (2013)
DOR	Doravirine	3.01	9.66	Triazolinone moiety	Chemsrc document and Drugbank Reference Doc
DLV	Delavirdine	2.98	4.5	Piperazine N & Methyl-sulfonamide group	Usach, et al. J Int AIDS Soc. 16(1): 18567. (2013)
ESV	Elsulfavirine	5.82	3.24	N-propanoyl sulfonamide	Drugbank Chemaxon

PIs (Protease Inhibitors)

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
LPV	Lopinavir	5.9	Null	Null	log P reference (Pubchem)
DRV	Darunavir	2.47	2.02	primary aniline nitrogen group	FDA Drug Evaluation Chart
ATV	Atazanavir	5.86	3.36, 4.88	-N in 2-phenylpyridine moiety, -OH alongside azapeptide backbone	Drugbank Sheet
RTV	Ritonavir	5.22	1.84, 2.77	thiazole N, secondary amine N	Human Metabolome Database
SQV	Saquinavir	3.16	8.47	Decahydroisoquinoline nitrogen	Drugbank sheet 1, Drugbank sheet 2
TPV	Tipranavir	7.14	4.43	4-hydroxy-2-pyrone	Drugbank sheet

Entry Inhibitors

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
MVC	Maraviroc	3.63	9.38	Tropane N	Human Metabolome Database
T20	Enfuvirtide (Fuzeon)	-14.7	3.86, 4.25, 6.00, 10.5	Aspartic acid side chain 1, Glutamic acid side chain 5, Histidine Side chain, Lysine side chain 2	Pubchem Data
FOS	Fostemsavir (Rukobia)	0.64	1.75,5.5	dihydrogen phosphate ester (1.75), Monohydrogen phosphate anion(5.5)	Drugbank
IBA	Ibalizumab* (Trogarzo)	Null	Null	Null	Highly polyprotic as humanized IgG4 monoclnal antibody with molecular size $\sim$ 15000 g/mol.

Capsid Inhibitor

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
LEN	Lenacapavir (Sunlenca)	3.4	6.4	Methanesulfonamide nitrogen	Drugbank sheet

INSTIs (Integrase Strand Transfer Inhibitors)

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
RAL	Raltegravir	1.06	6.70	enolic hydroxyl group (-OH)	Invivochem documentation
DTG	Dolutegravir	2.2	8.2	hydroxypyrimidinone N–OH (chelating pharmacophore)	Therapeutic Goods Association Documentation
CAB	Cabotegravir	1.04	7.8	Enolic Hydroxyl group -OH	FDA Documentation
EVG	Elvitegravir	4.98	6.5	Quinolone carboxylic acid –COOH	Pubmed Documentation
BIC	Bictegravir	9.81	1.36	Enolic hydroxyl oxygen -OH	Drugbank Chemaxon

CYP3A4 Pharmacokinetic Boosters

Drug	Full Name	log P	pKa(s)	Ionizable Group(s)	Note
COB	Cobicistat	4.3	6.4	Morpholine N	Gilead Science Official doc