

Type of Calculation	AveErr	RMS	AUE	tau	R	maxErr	percent correct sign	error slope
LogD_calc	1.6 +/- 0.3	2.6 +/- 0.2	2.1 +/- 0.2	0.49 +/- 0.08	0.6 +/- 0.1	5.5 +/- 0.3	70 +/- 6	0.63 +/- 0.08
LogD_oneCorrected	0.7 +/- 0.3	2.4 +/- 0.2	2.0 +/- 0.2	0.65 +/- 0.07	0.78 +/- 0.07	7 +/- 1	75 +/- 6	0.62 +/- 0.07
LogD_acidCorrected	1.0 +/- 0.3	2.6 +/- 0.2	2.2 +/- 0.2	0.58 +/- 0.08	0.75 +/- 0.08	6.6 +/- 0.7	75 +/- 6	0.59 +/- 0.08
LogD_baseCorrected	1.3 +/- 0.3	2.4 +/- 0.2	2.0 +/- 0.2	0.53 +/- 0.08	0.7 +/- 0.1	5.5 +/- 0.4	70 +/- 6	0.66 +/- 0.07
limited logP largestpKa	1.9 +/- 0.4	3.0 +/- 0.3	2.5 +/- 0.3	0.5 +/- 0.1	0.6 +/- 0.2	5.5 +/- 0.3	59 +/- 8	0.19 +/- 0.07
limited logD largestpKa	0.5 +/- 0.5	2.7 +/- 0.3	2.3 +/- 0.2	0.66 +/- 0.09	0.7 +/- 0.1	7 +/- 1	68 +/- 8	0.08 +/- 0.05
limited logP basicpKa	2.1 +/- 0.3	2.7 +/- 0.3	2.4 +/- 0.3	0.6 +/- 0.1	0.79 +/- 0.09	5.4 +/- 0.6	65 +/- 9	0.15 +/- 0.07
limited logD basicpKa	1.4 +/- 0.4	2.3 +/- 0.2	2.1 +/- 0.2	0.71 +/- 0.09	0.81 +/- 0.07	3.7 +/- 0.3	65 +/- 9	0.010 +/- 0.06
limited logP acidipKa	1.6 +/- 0.8	3.2 +/- 0.5	2.5 +/- 0.6	0.0 +/- 0.3	0.3 +/- 0.5	5.5 +/- 0.5	50 +/- 10	0.3 +/- 0.1
limited logD acidipKa	-0.8 +/- 0.9	3.2 +/- 0.5	2.6 +/- 0.5	0.4 +/- 0.2	0.6 +/- 0.3	7 +/- 1	80 +/- 10	0.2 +/- 0.1
all LogD Klamt	0.5 +/- 0.3	2.1 +/- 0.2	1.7 +/- 0.2	0.73 +/- 0.04	0.84 +/- 0.04	6.1 +/- 0.8	79 +/- 6	0.46 +/- 0.07