

ID	name	K_a (M^{-1})	ΔG (kcal/mol) ^(a)	ΔH (kcal/mol)	$T\Delta S$ (kcal/mol) ^(b)	n
CB8-G1	Methamphetamine ^(c)	150000.0 +- 10000.0	-7.05 +- 0.04	-7.8 +- 0.3	-0.8 +- 0.3	1.00
CB8-G2	Fentanyl ^(c)	19000000.0 +- 1000000.0	-9.93 +- 0.03	-10.8 +- 0.3	-0.9 +- 0.3	1.00
CB8-G3	Morphine ^(d)	340000000.0 +- 20000000.0	-11.63 +- 0.03	-13.6 +- 0.4	-2.0 +- 0.4	1.00
CB8-G4	Hydromorphone ^(d)	170000000.0 +- 10000000.0	-11.22 +- 0.04	-15.8 +- 0.5	-4.6 +- 0.5	1.00
CB8-G5	Ketamine ^(e)	1090000000.0 +- 80000000.0	-12.32 +- 0.04	-17.3 +- 0.5	-5.0 +- 0.5	1.00
CB8-G6	PhenylCyclohexylPiperidine(PCP) ^(e)	21000000000.0 +- 2000000000.0	-14.07 +- 0.06	-14.9 +- 0.4	-0.8 +- 0.5	1.00
CB8-G7	Cocaine ^(c)	640000.0 +- 50000.0	-7.92 +- 0.04	-8.3 +- 0.3	-0.3 +- 0.3	1.00

All quantities are reported as point estimate +- statistical error from the ITC data fitting procedure. The upper bound (1%) was used for errors reported to be < 1%. We also included a 3% relative uncertainty in the titrant concentration assuming the stoichiometry coefficient to be fitted to the ITC data for the Isaacs (CB8) dataset, where concentration error had not been factored in to the original error estimates..

^(a) Statistical errors were propagated from the K_a measurements.

^(b) All experiments were performed at 298 K.

^(c) Direct ITC titration.

^(d) Competitive ITC titration with C1.

^(e) Competitive ITC titration with C2.