

## DB params compare

CAS	Chemical	Type of Observation	MW	H_UNITS	H_PRIME	DENSITY	DIA	DIW	KOC	S	RAGSE_ABS	RAGSE_GIABS
000000-06-6	Vanadium and Compounds	Spring 2012	50.94							0		1
		Fall 2012	50.94			6						1
		Change Effect										
000053-96-3	Acetylaminofluorene, 2-	Spring 2012	223.28	1.92E-10	7.8496E-09		0.051624	6.0319E-06	2206	0	0.1	1
		Fall 2012	223.28	1.92E-10	7.8496E-09		0.051624	6.0319E-06	2206	8.4607	0.1	1
		Change Effect									8.4607	
000074-31-7	N,N'-Diphenyl-1,4-benzenediamine	Spring 2012	260.34	2.05E-10	8.381E-09		0.046601	5.4449E-06	51890	0	0.1	1
		Fall 2012	260.34	2.05E-10	8.381E-09		0.046601	5.4449E-06	51890	1.5867	0.1	1
		Change Effect									1.5867	
000092-87-5	Benzidine	Spring 2012	184.24	7.05E-11	2.8823E-09	1.219	0.058681	6.8564E-06	1190	322	0.1	1
		Fall 2012	184.24	7.05E-11	2.8823E-09	1.219	0.035127	7.4756E-06	1190	322	0.1	1
		Change Effect					-0.023554					
000094-59-7	Safrole	Spring 2012	162.19	0.00000907	0.0003708	1.1	0.044227	7.5874E-06	207.2	0	0.1	1
		Fall 2012	162.19	0.00000907	0.0003708	1.1	0.044227	7.5874E-06	207.2	5.8996	0.1	1
		Change Effect									5.8996	
000102-76-1	Triacetin	Fall 2012	218.21	1.23E-08	5.03E-07	1.1583	0.02558	0.00000655	40.73	58000	0.1	1
000107-07-3	Chloroethanol, 2-	Fall 2012	80.51	7.61E-07	0.0000311	1.2019	0.099986	0.0000122	1.904	1000000	0.1	1
000110-83-8	Cyclohexene	Fall 2012	82.15	0.0455	1.8601799		0.100542	0.0000117	145.8	213		1
000127-63-9	Diphenyl Sulfone	Spring 2012	218.27	2.49E-07	0.0000102	1.252	0.026518	6.8618E-06	1109	0	0.1	1
		Fall 2012	218.27	2.49E-07	0.0000102	1.252	0.026518	6.8618E-06	1109	9.4191	0.1	1
		Change Effect									9.4191	
000193-39-5	Indeno[1,2,3-cd]pyrene	Spring 2012	276.34	3.48E-07	0.0000142		0.044784	5.2327E-06	1951000	0.00019	0.13	1
		Fall 2012	276.34	1.6046E-06	0.0000656		0.044784	5.2327E-06	3470000	0.000022	0.13	1
		Change Effect								1519000	-0.000168	
000301-04-2	Lead acetate	Spring 2012	325.29			3.25	0.033366	9.5728E-06	1	1600	0.1	1
		Fall 2012	325.29			3.25	0.033366	9.5728E-06	1	443000	0.1	1
		Change Effect									441400	
000460-19-5	Cyanogen	Spring 2012	52.04	0.0054	0.2207686	0.9537	0.123753	0.0000138		4500000		1
		Fall 2012	52.04	0.0054	0.2207686	0.9537	0.123753	0.0000138		9487		1
		Change Effect									-4490513	
000463-56-9	Thiocyanate	Spring 2012	59.09	0.000146	0.0059689		0.12524	0.0000146	4.67	35319		1
		Fall 2012	59.09				0.12524	0.0000146				1
		Change Effect										
000506-77-4	Cyanogen Chloride	Spring 2012	61.47	0.0019412	0.0787186	1.186	0.120745	0.0000142		25000000		1
		Fall 2012	61.47	0.0019412	0.0787186	1.186	0.120745	0.0000142		30000		1
		Change Effect									-24970000	
000593-60-2	Vinyl Bromide	Spring 2012	106.95	0.0123	0.5028618	1.4933	0.086224	0.0000117	21.73	0		1
		Fall 2012	106.95	0.0123	0.5028618	1.4933	0.086224	0.0000117	21.73	10358		1
		Change Effect									10358	
000636-21-5	Methylaniline Hydrochloride, 2	Spring 2012	107.16	0.00000198	0.0000809		0.084217	9.8401E-06	115	16600	0.1	1
		Fall 2012	143.62	0.00000198	0.0000809		0.06928	8.0949E-06	115	16600	0.1	1
		Change Effect					-0.014936					
000680-31-9	Hexamethylphosphoramide	Spring 2012	179.2	7.13E-12	2.92E-10		0.059776	6.9844E-06	10	1000000	0.1	1
		Fall 2012	179.2	7.13E-12	2.92E-10	1.03	0.034837	6.8702E-06	10	1000000	0.1	1
		Change Effect					-0.024939					
001163-19-5	Decabromodiphenyl ether, 2,2',3,3',4,4',5,5',6,6'- (BDE-209)	Spring 2012	959.17	4.45E-08	1.8193E-06	3	0.019535	2.2826E-06	276200	0.0001	0.1	1
		Fall 2012	959.17	4.45E-08	1.8193E-06	3	0.018924	4.7688E-06	276200	0.0001	0.1	1
		Change Effect					-0.000611					
001335-32-6	Lead subacetate	Spring 2012	805.7				0.021943	2.5639E-06	10.37	62500	0.1	1

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	Lead subacetate	Fall 2012	805.7				0.021943	2.5639E-06	10.37	63000	0.1	1
		Change Effect								500		
003165-93-3	Chloro-2-methylaniline HCl, 4-	Spring 2012	141.6	0.00000199	0.0000814		0.069938	8.1717E-06	184.5	1732.4	0.1	1
	Chloro-2-methylaniline HCl, 4-	Fall 2012	178.06	1.44E-13	5.887E-12		0.060031	7.0142E-06	351.9	115.68	0.1	1
		Change Effect	36.46				-0.009907		167.4	-1616.72		
004170-30-3	Crotonaldehyde	Spring 2012	70.09	0.0000194	0.0007931	0.853	0.095993	0.0000108	1.793	181000	0.1	1
	Crotonaldehyde	Fall 2012	70.09	0.0000194	0.0007931	0.853	0.095993	0.0000108	1.793	180000	0.1	1
		Change Effect								-1000		
007773-06-0	Ammonium Sulfamate	Spring 2012	97.09							147000		1
	Ammonium Sulfamate	Fall 2012	114.124							147000		1
		Change Effect	17.034									
010294-34-5	Boron Trichloride	Fall 2012	117.17			4.789						1
013674-84-5	Tris(1-chloro-2-propyl)phosphate	Fall 2012	327.57	5.96E-08	0.00000244		0.039984	4.6718E-06	1604	1200	0.1	1
021436-96-4	Dimethylaniline HCl, 2,4-	Spring 2012	121.18	0.0000025	0.0001022		0.077589	9.0657E-06	184.5	2175.5	0.1	1
	Dimethylaniline HCl, 2,4-	Fall 2012	157.64	2.15E-13	8.79E-12		0.065109	7.6075E-06	351.9	150.28	0.1	1
		Change Effect	36.46		-0.000102		-0.01248		167.4	-2025.22		
025013-15-4	Methyl Styrene (Mixed Isomers)	Spring 2012	118.18	0.00255	0.1042518		0.078897	9.2184E-06	697.8	89		1
	Methyl Styrene (Mixed Isomers)	Fall 2012	118.18	0.00301	0.1230581		0.078897	9.2184E-06	715.8	89		1
		Change Effect		0.00046	0.0188062				18			