Question 1 - please consult 1(a) for the appropriate formulae

a)

logKow

Fragment	Number	Constant	Contribution
fC(aromatic)	12	0.13	1.56
fC(aliphatic)	4	0.2	0.8
fH	15	0.23	3.45
fO (aromatic)	2	-0.61	-1.22
fCl(aliphatic)	3	0.06	0.18
fch	1	(6-1)(-0.12)	-0.6
	2	(2-1)(-0.12)	-0.24
fpolyhalo	1	1.59	1.59
		Total	**5.52**

* branching should be included and was accepted in answers

C^{sat}_{w}

type	substituted benzene, polar
a	0.72
b	1.18
logKow	5.52
MW	344.65
C^{sat}_{w} (ppm)	**1.28E-1**

C^{sat}_{w} (mol/m^3) = 1/10^[(logKow-b)/a)] = 10^[(b-logKow)/a)]

C^{sat}_{w} (ppm) = C^{sat}_{w} (mol/m^3) * MW (g/mol) (since 1 ppm = 1 g/m^3)

*substituted benzene, non-polar; miscellaneous pesticide were also acceptable

*several students took the approach of converting Kow to Kom, then Kom to Csat/w. This approach was not penalized but the above approach is encouraged on the final exam.

VP

Fragment	Number	Constant	Contribution
=CH-	8	-0.46	-3.68
=CX-	4	-0.63	-2.52
X-CCl3	1	-1.89	-1.89
X-CH-R2	1	-0.19	-0.19
X-O-Ar	2	-0.7	-1.4
X-CH3	2	-0.28	-0.56
		Total	-10.24

VP (Pa) = 10^(-10.24-(1.56*(87-25))/100+4.42)*101325/760 = **2.18E-5 Pa**

Kaw

Kaw = H/RT = (P/C^{sat}_{w})/RT = [(2.18E-5 Pa)/(1.28E-1 g/m^3)*(344.65 g/mol)] / (8.314*298)
= 2.37E-5

b)

logKow

Fragment	Number	Constant	Contribution
fC(aromatic)	6	0.13	0.78
fC(aliphatic)	2	0.2	0.4
fH	10	0.23	2.3
fN(H)C(O)N (aromatic)	1	-2.29	-2.29
fCl(aromatic)	1	0.94	0.94
fch	1	(3-1)(-0.12)	-0.24
fbr nonpolar	1	-0.13	-0.13
		Total	**1.76**

C^{sat}_{w}

type	substituted benzene, polar
a	0.72
b	1.18
logKow	1.76
MW	198.659
C^{sat}_{w} (ppm)	**1.40E+04**

*also accepted miscellaneous pesticide

VP

Fragment	Number	Constant	Contribution
=CH-	4	-0.46	-1.84
=CX-	2	-0.63	-1.26
X-Cl	1	-0.53	-0.53
X-NHCONR2	1	-6.47	-6.47
X-CH3	2	-0.28	-0.56
		Total	**-10.66**

VP (Pa) = 10^(**-10.66**-(1.56*(180-25))/100+4.42)*101325/760 = 2.93E-7 Pa

Kaw

Kaw = 1.68E-12

c)

logKow

Fragment	Number	Constant	Contribution
fC(aliphatic)	5	0.2	1
fH	2	0.23	0.46
fF(aliphatic)	10	-0.38	-3.8
fO(aliphatic)	1	-1.82	-1.82
fpoly(2same)	2	0.6	1.2
fpoly(3same)	2	1.59	3.18
fadj(4)	1	0.84	0.84
fadj(5)	1	1.12	1.12
fch	1	(15-1)(-0.12)	-1.68
		Total	**0.5**

C^{sat}_w

type	alkane
a	0.81
b	-0.2
logKow	0.5
MW	268.05
C^{sat}_w (ppm)	**8.85E+05**

VP

Fragment	Number	Constant	Contribution
X-CF3	2	-0.2	-0.4
X-F2	2	-0.33	-0.66
X-CH2-R	1	-0.45	-0.45
X-O-R	1	-0.43	-0.43
		Total	-1.94

VP (Pa) = 10^(-1.94-(1.56*(0))/100+4.42)*101325/760 = **4.03E-4 Pa**

*also use of XCR3 and 2*XF was acceptable, in lieu of each XF2

Kaw

Kaw = 4.93E-3

d)

Kow

Fragment	**Number**	**Constant**	**Contribution**
Fragment Type	#	Constant	Contribution
fC(aromatic)	6	0.13	0.78
fC(aliphatic)	2	0.2	0.4
fH	10	0.23	2.3
festerCOO(aromatic)	2	-0.56	-1.12
fch	2	(2-1)(-0.12)	-0.24
fnearby polar	1	-0.16(-0.56-0.56)	0.1792
		Total	**2.2992**

C^{sat}_{w}

type	phthalate
a	1.06
b	-0.22
logKow	2.2992
MW	194.18
C^{sat}_{w} (ppm)	**8.14E+02**

VP

Fragment	**Number**	**Constant**	**Contribution**
=CH-	4	-0.46	-1.84
=CX-	2	-0.63	-1.26
X-COOR	2	-1.19	-2.38
X-CH3	2	-0.28	-0.56
		Total	-6.04

VP (Pa) = 10^(**-6.04** -(1.56*(0))/100+4.42)*101325/760 = **3.20 Pa**

*inclusion 6-25 as “melting” term was also accepted

Kaw

Kaw = 3.08E-4

e)

Kow

Fragment	Number	Constant	Contribution
fC(aromatic)	12	0.13	1.56
fH	2	0.23	0.46
fBr(aromatic)	8	1.09	8.72
fO(2aromatic)	1	0.53	0.53
fch	1	(2-1)(-0.12)	-0.12
		Total	**11.15**

C^{sat}_w

type	substituted benzene, polar
a	0.72
b	1.18
logKow	11.15
MW	801.38
C^{sat}_w (ppm)	**1.34E-08**

*substituted benzene, non-polar and PCB were also accepted

VP

Fragment	Number	Constant	Contribution
=CH-	2	-0.46	-0.92
=CX-	10	-0.63	-6.3
X-Br	8	-0.84	-6.72
X-O-Ar	1	-0.33	-0.33
		Total	-14.27

VP (Pa) = 10^(-14.27-(1.56*(200-25))/100+4.42)*101325/760 = **3.51E-11 Pa**

Kaw

Kaw = 8.48E-4

f)

logKow

Fragment	Number	Constant	Contribution
fC(aromatic)	6	0.13	0.78
fC(aliphatic)	1	0.2	0.2
fH	5	0.23	1.15
fNO2 (aromatic)	3	-0.03	-0.09
fnearby polar	3	-0.08(-0.03-0.03)	0.0144
		Total	**2.0544**

C^{sat}_w

type	substituted benzene, polar
a	0.72
b	1.18
logKow	2.0544
MW	227.15
C^{sat}_w (ppm)	**1.39E4**

VP

Fragment	Number	Constant	Contribution
=CH-	2	-0.46	-0.92
=CX-	4	-0.63	-2.52
X-CH3	1	-0.34	-0.34
X-NO2	3	-1.45	-4.35
		Total	**-8.13**

VP (Pa) = 10^(**-8.13**-(1.56*(L10-25))/100+4.42)*101325/760 = **3.48E-3 Pa**

Kaw

Kaw = 2.30E-8

Question 2

logKow

Fragment	Number	Constant	Contribution
fC(aromatic)	12	0.13	1.56
fC	1	0.2	0.2
fH	7	0.23	1.61
fBr(aromatic)	5	1.09	5.45
fO(2aromatic)	1	0.53	0.53
fO(aromatic)	1	-0.61	-0.61
fch	2	(2-1)(-0.12)	-0.24
fpolar	1	-0.16*(0.53-0.61)	0.0128
		Total	**8.51**

logBCF = 0.76*logKow - 0.23 = 6.240

BCF = 1.74E6

concentration in fish = 34.7 ppm

density of fish = 1 (or reasonable assumption)

mass in fish = 3.47 mg

logKom = 0.82*logKow + 0.14 = 7.120

Kom = 1.32E7

Koc = 2.64E7

logKoc = 7.42

Kd = 5.28E5

concentration in sediment = 10.6 ppm

Question 3

		Compound		MW (g/mol)	VP (Pa)	C_w^{sat} (g/m^3)	$\log K_{ow}$	K_{aw}	K_{ow}	mole fraction in water	mole fraction in air	mole fraction in octanol
Volumes (m^3)		Benzene	A	78.1	12700	1780	2.13	0.22	1.35E+02	0.043	0.957	0.0000
Vair	100000000	Toluene	B	92.13	3800	515	2.69	0.27	4.90E+02	0.035	0.965	0.0000
Vwater	1000000	p-xylene	C	106.2	1170	215	3.18	0.23	1.51E+03	0.041	0.959	0.0001
Voctanol	1	Chlorobenzene	D	112.6	1580	484	2.8	0.15	6.31E+02	0.063	0.937	0.0000
		1,2,3 Trichlorobenzene	E	181.45	28	21	4.1	0.10	1.26E+04	0.093	0.906	0.0012
Constants		Dioctyl phthalate	F	390.6	0.187	0.02	6	1.47	1.00E+06	0.007	0.987	0.0067
R (Pa*m^3/mol/K)	8.314	2,4,6 trichlorophenol	G	197.45	1.25	434	3.69	0.00	4.90E+03	0.973	0.022	0.0048
T (K)	298.15	Pentachlorobenzene	H	250.3	0.22	0.65	5	0.03	1.00E+05	0.221	0.757	0.022
n (mol)	1	Pyrene	I	202.3	0.0006	0.132	5.18	0.00	1.51E+05	0.841	0.031	0.127
		2,2',4,4',6,6'-hexachlorobiphenyl	J	360.9	0.00048	0.002	7	0.03	1.00E+07	0.069	0.241	0.690

		Hexachlorobenzene		**MW (g/mol)**	**VP (Pa)**	**C_w^{sat} (g/m^3)**	**logK_{ow}**	**K_{aw}**	**K_{ow}**	**mole fraction in water**	**mole fraction in air**	**mole fraction in octanol**
T (K)	287.95	14.8	A	284.8	0.000611	0.00705	5.5	0.01031	316227.8	0.19	0.20	0.61
	293.25	20.1	B	284.8	0.0011	0.00886	5.5	0.014503	316227.8	0.18	0.26	0.56
	295.25	22.1	C	284.8	0.00136	0.00959	5.5	0.016454	316227.8	0.17	0.28	0.54
	297.35	24.2	D	284.8	0.0017	0.0104	5.5	0.018831	316227.8	0.17	0.31	0.52
	307.95	34.8	E	284.8	0.00499	0.0158	5.5	0.035131	316227.8	0.13	0.46	0.41
	323.65	50.5	F	284.8	0.0216	0.0277	5.5	0.082533	316227.8	0.08	0.66	0.25

Volumes (m^3)	
Vair	10000000
Vwater	100000
Voctanol	1
Constants	
R (Pa*m^3/mol/K)	8.314
n (mol)	1