SMILES	c1c3c2c(cc1)cc5c4c2c(cc3)cc6c4c(cc5)ccc6		C_w= 0.000
Compound No.	11109		C_g= 0.000
Compound Name	**Dibenzo[cd,jk]pyrene**		**log Kw=** #DIV/0!
Molecular Formula	C22H12		P + L, count: 7
Molecular weight	276.3300	**WS (mg/L)=**	
CAS No	191-26-4	**VP (mm Hg)=**	**P+L, sd: 0.023**
ACD/n20 =	2.009		
E =	5.106		Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)	
7.040	6.584	6.584	7.29	6.89	**P+L, sd(W): 0.023**

UNIX	SMART			PA	
4.17	4.621	logKw	6.927		P, count: 1
2.09		R (**E**)=	**4.621**	3.92	
0.00	0.00	Pi (**S**)=	2.100	2.02	**P, sd: #DIV/0!**
0.40		Alpha (**A**) =	**0.000**	0.00	
13.19	13.234	Beta (**B**)=	0.400	0.33	L, count: 6
		LogL16 (**L**) =	13.203	12.889	
		Vx (**V**)=	2.0838		**L, sd: 0.025**

LogPcalc	LogPobs
7.035	7.040

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	LogPcalc	LogPcalc	LogPobs	(Po-Pc)^2	
	Octanol	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814	P	Octanol (wet)	7.035	7.035	7.040	0.000	P*
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	7.151	na		na	

											logL(calc)	logL(calc)	logL(obs)	
MHA unpub.	Octanol/Wet/March 98	-0.198	0.002	0.709	3.519	1.429	0.858	0.000	L	Octanol/Wet/March 98	13.200	na		na
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	7.401	na		na
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	13.203	13.203	13.234	0.001
Anal Chem (1988)	DB-5	0.097	0.000	0.252	-2.480	0.000	0.337	0.000	RI/100	DB-5	5.075	5.075	5.053	0.000
J Chromatog (1992	SE-54	0.094	0.000	0.261	-2.480	0.000	0.333	0.000	RI/100	SE-54	5.039	5.039	5.065	0.001
Chemosphere (199	HP-5	0.074	0.000	0.256	0.000	0.000	0.338	0.000	RI/100	HP-5	5.074	5.074	5.049	0.001
Environ Toxicol Ch	DB-5	0.110	0.000	0.244	-3.061	-0.244	0.344	0.000	RI/100	DB-5	5.067	5.067	5.084	0.000
J Gas Chromatog (	SE-52	-1.081	0.860	0.000	0.000	0.000	2.195	0.000	RI/100	SE-52	31.874	31.874	31.860	0.000