SMILES	c1cccc2c1CCC(O2)=O			C_w=	
Compound No.	18621			C_g=	
Compound Name	**Dihydrocoumarin**			**log Kw=**	
Molecular Formula	C9H8O2			P + L, count:	11
Molecular weight	148.1600	**WS (mg/L)=**			
CAS No	119-84-6	**VP (mm Hg)=**		**P+L, sd:**	**0.082**
S-A/n20 =	1.556				
E =	0.948			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	1.630	1.626	1.53	1.80	**P+L, sd(W):**	**0.082**

UNIX	SMART			PA		
1.14	0.950	logKw	4.836		P, count:	3
1.70		R (**E**)=	**0.948**	0.96		
0.00	0.00	Pi (**S**)=	1.670	1.79	**P, sd:**	**0.064**
0.57		Alpha (**A**) =	**0.000**	0.00		
6.13		Beta (**B**)=	0.420	0.54	L, count:	8
		LogL16 (**L**) =	5.632	6.005		
		Vx (**V**)=	1.1049		**L, sd:**	**0.092**

LogPcalc	LogPobs
2.459	2.421

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)	1.621	1.621	1.630	0.000	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	0.872	0.872	0.796	0.006	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.883	4.883	4.836	0.002	
											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	6.420	6.420	6.466	0.002	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	5.632	5.632	5.632	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.911	4.911	4.836	0.006	
Botanica Complute	DB-1	0.555	0.000	0.906	1.847	0.000	1.997	0.000	RI/100	DB-1	13.314	13.314	13.370	0.003	
Flav Frag J (2006)	HP-101	0.801	-0.264	1.739	3.144	-1.233	1.978	0.000	RI/100	HP-101	14.076	14.076	13.920	0.024	
"Qual Anal Flav Fra	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	22.346	na		na	22.860
"Qual Anal Flav Fra	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	13.848	na		na	13.590
Anal Chem (1993)	OV-101	0.426	-0.311	1.145	1.189	0.000	2.034	0.000	RI/100	OV-101	13.498	13.498	13.590	0.008	
Anal Chem (1993)	CW-20M	0.249	1.200	6.184	8.439	-0.765	2.027	0.000	RI/100	CW-20M	22.808	22.808	22.860	0.003	
	Supelco-Wax TM10	0.127	0.000	6.664	9.249	0.000	2.034	0.000	RI/100	Supelco-Wax TM10	22.710	na		na	23.140
	HP-1	0.557	-0.770	1.501	1.252	0.000	2.003	0.000	RI/100	HP-1	13.614	13.614	13.500	0.013	