SMILES	C=CCC=C		C_w= **0.008**
Compound No.	1200		C_g= 0.040
Compound Name	**Penta-1,4-diene**		**log Kw=** -0.691
Molecular Formula	C5H8		P + L, count: 14
Molecular weight	68.1170	**WS (mg/L)=** 558	
CAS No	591-93-5	**VP (mm Hg)=** 748	**P+L, sd: 0.046**
S-A/n20 =	1.389		
E =	**0.186**		Weight: 1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
2.470	2.37	2.371	2.48	2.39	**P+L, sd(W): 0.046**

UNIX	**SMART**			**PA**	
0.40	0.185	logKw	**-0.691**		P, count: 3
0.21	0.14	R (**E**)=	**0.186**	0.25	
0.00	0.00	Pi (**S**)=	0.170	0.30	**P, sd: 0.049**
0.14	0.10	Alpha (**A**) =	**0.000**	0.00	
2.04	1.998	Beta (**B**)=	0.090	0.14	L, count: 11
		LogL16 (**L**) =	1.974	2.116	
		Vx (**V**)=	**0.7271**		**L, sd: 0.048**

LogPcalc	LogPobs
1.516	1.481

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)	2.475	2.475	2.470	0.000	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.721	2.721	2.665	0.003	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.650	-0.650	-0.691	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	1.745	1.745	1.779	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.639	-0.639	-0.691	0.003	
Bull Soc Chim Fr	Squalene	0.888	-1.550	2.169	1.834	0.000	1.915	0.000	RI/100	Squalene	4.749	4.749	4.710	0.002	
Bull Soc Chim Fr	Dimethylsulfolane	0.862	1.587	3.804	8.466	1.683	1.940	0.000	RI/100	Dimethylsulfolane	5.785	5.785	5.880	0.009	
J Chrom Sci (197	Squalene	0.781	-0.736	1.085	0.000	0.000	1.947	0.000	RI/100	Squalene	4.672	4.672	4.621	0.003	
J HRC&CC (1982)	SE-30	0.739	0.000	0.489	1.168	1.009	1.954	0.000	RI/100	SE-30	4.771	4.771	4.800	0.001	
J HRC&CC (1982)	SE-30	0.761	0.339	0.466	1.711	0.000	1.973	0.000	RI/100	SE-30	4.798	na		na	4.610
Ing Eng Chem Pro	Squalene	0.703	0.000	0.299	0.000	0.000	1.981	0.000	RI/100	Squalene	4.665	4.665	4.622	0.002	
Ing Eng Chem Pro	Squalene	0.721	0.000	0.666	0.000	-1.095	1.987	0.000	RI/100	Squalene	4.659	4.659	4.625	0.001	
Ing Eng Chem Pro	Squalene	0.758	-0.295	0.769	0.000	-0.683	1.971	0.000	RI/100	Squalene	4.664	4.664	4.638	0.001	
Ing Eng Chem Pro	Squalene	0.732	0.000	0.547	0.000	-0.838	1.978	0.000	RI/100	Squalene	4.655	4.655	4.643	0.000	
	SUPELCO PETROCO	0.712	0.000	0.434	1.113	0.484	1.995	0.000	RI/100	SUPELCO PETROCOL D	4.768	4.768	4.805	0.001	