SMILES	C=CCCC=C			C_w=	**0.002**
Compound No.	1226			C_g=	0.012
Compound Name	**Hexa-1,5-diene**			**log Kw=**	-0.762
Molecular Formula	C6H10			P + L, count:	15
Molecular weight	82.1436	**WS (mg/L)=**	169		
CAS No	592-42-7	**VP (mm Hg)=**	221	**P+L, sd:**	**0.059**
S-A/n20 =	1.404				
E =	**0.190**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
2.870	**2.900**	2.900	2.82	2.80	**P+L, sd(W):**	**0.059**

UNIX	**SMART**			**PA**		
		logKw	**-0.762**		P, count:	4
0.40	0.191	R (**E**)=	**0.190**	0.25		
0.21	0.15	Pi (**S**)=	0.210	0.31	**P, sd:**	**0.077**
0.00	0.00	Alpha (**A**) =	**0.000**	0.00		
0.14	0.10	Beta (**B**)=	0.090	0.14	L, count:	11
2.54	2.450	LogL16 (**L**) =	2.463	2.610		
		Vx (**V**)=	**0.8680**		**L, sd:**	**0.056**

											LogPcalc	LogPobs		
											2.316	2.258		
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)	2.973	2.973	2.900	0.005	CLOGP
CTET-1	Tetrachloromethane	0.260	0.573	-1.254	-3.558	-4.588	0.000	4.589	P	CCl4 Sept 98	3.676	3.676	3.670	0.000	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	3.284	3.284	3.225	0.004	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.668	-0.668	-0.762	0.009	

											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	2.193	2.193	2.138	0.003	
CTET-1	Tetrachloromethane	0.282	-0.303	0.460	0.000	0.000	1.047	0.000	L	CCl4/Sept 98	2.899	2.899	2.908	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.630	-0.630	-0.762	0.017	
Bull Soc Chim Fr	Squalene	0.888	-1.550	2.169	1.834	0.000	1.915	0.000	RI/100	Squalene	5.765	5.765	5.760	0.000	
Bull Soc Chim Fr	Dimethylsulfolane	0.862	1.587	3.804	8.466	1.683	1.940	0.000	RI/100	Dimethylsulfolane	6.891	6.891	6.980	0.008	
J HRC&CC (1982)	SE-30	0.739	0.000	0.489	1.168	1.009	1.954	0.000	RI/100	SE-30	5.744	5.744	5.750	0.000	
J HRC&CC (1982)	SE-30	0.761	0.339	0.466	1.711	0.000	1.973	0.000	RI/100	SE-30	5.782	5.782	5.750	0.001	
Ing Eng Chem Prc	Squalene	0.703	0.000	0.299	0.000	0.000	1.981	0.000	RI/100	Squalene	5.644	5.644	5.628	0.000	
Ing Eng Chem Prc	Squalene	0.721	0.000	0.666	0.000	-1.095	1.987	0.000	RI/100	Squalene	5.655	5.655	5.627	0.001	
Ing Eng Chem Prc	Squalene	0.758	-0.295	0.769	0.000	-0.683	1.971	0.000	RI/100	Squalene	5.656	5.656	5.628	0.001	
Ing Eng Chem Prc	Squalene	0.732	0.000	0.547	0.000	-0.838	1.978	0.000	RI/100	Squalene	5.642	5.642	5.633	0.000	
Report of Hydroca	SUPELCO PETROCO	0.712	0.000	0.434	1.113	0.484	1.995	0.000	RI/100	SUPELCO PETROCOL [	5.759	na		na	5.633