SMILES	C(C=C=C)C			C_w=	**0.000**
Compound No.	1170			C_g=	0.000
Compound Name	**1,2-Pentadiene**			**log Kw=**	#DIV/0!
Molecular Formula	C5H8			P + L, count:	14
Molecular weight	68.1170	**WS (mg/L)=**			
CAS No	591-95-7	**VP (mm Hg)=**		**P+L, sd:**	**0.029**
ACD/n20 =	1.391				
E =				Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	2.430	2.431	2.37	2.50	**P+L, sd(W):**	**0.029**

UNIX	**SMART**			**PA**		
0.31	0.310	logKw	-0.341		P, count:	3
0.21		R (**E**)=	**0.310**	**0.20**		
0.00	0.00	Pi (**S**)=	0.230	**0.31**	**P, sd:**	**0.016**
0.14		Alpha (**A**) =	**0.000**	**0.00**		
1.98		Beta (**B**)=	0.110	**0.12**	L, count:	11
		LogL16 (**L**) =	2.273	**2.034**		
		Vx (**V**)=	**0.7271**		**L, sd:**	**0.033**

											LogPcalc	LogPobs		
											1.565	1.568		
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)	2.412	2.412	2.431	0.000	CLOGP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.610	2.610	2.614	0.000	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.328	-0.328	-0.341	0.000	

											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	2.073	2.073	2.090	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	2.273	2.273	2.273	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.340	-0.340	-0.341	0.000
Chromatographia	Squalene	0.649	-0.229	0.624	0.000	-0.495	2.010	0.000	RI/100	Squalene	5.236	5.236	5.256	0.000
Chromatographia	Squalene	0.627	-0.193	0.698	0.000	-0.740	2.024	0.000	RI/100	Squalene	5.247	5.247	5.259	0.000
Chromatographia	Citroflex	0.720	-0.707	3.164	0.000	1.627	1.997	0.000	RI/100	Citroflex	5.947	5.947	5.985	0.001
Chromatographia	Citroflex	0.688	-0.657	3.187	0.000	1.378	2.013	0.000	RI/100	Citroflex	5.944	5.944	5.972	0.001
Bull Soc Chim Fr	Squalene	0.888	-1.550	2.169	1.834	0.000	1.915	0.000	RI/100	Squalene	5.259	5.259	5.270	0.000
Bull Soc Chim Fr	Dimethylsulfolane	0.862	1.587	3.804	8.466	1.683	1.940	0.000	RI/100	Dimethylsulfolane	6.824	6.824	6.750	0.005
Ind Eng Chem Prc	Squalene	0.758	-0.295	0.769	0.000	-0.683	1.971	0.000	RI/100	Squalene	5.248	5.248	5.250	0.000
Ind Eng Chem Prc	Squalene	0.732	0.547	0.000	0.000	-0.838	1.978	0.000	RI/100	Squalene	5.305	5.305	5.260	0.002