SMILES	C\C(=C\C=C)C			C_w=	0.000
Compound No.	1186			C_g=	0.000
Compound Name	**4-Methyl-1,3-pentadiene**			**log Kw=**	#DIV/0!
Molecular Formula	C6H10			P + L, count:	16
Molecular weight	82.1400	**WS (mg/L)=**			
CAS No	926-56-7	**VP (mm Hg)=**		**P+L, sd:**	**0.053**
Beil/n20 =	1.449				
E =	**0.396**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	2.830	2.830	2.59	2.94	**P+L, sd(W):**	**0.053**

UNIX	**SMART**			**PA**		
0.41	0.405	logKw	-0.254		P, count:	2
0.25		R (**E**)=	**0.396**	0.26		
0.00	0.00	Pi (**S**)=	0.270	0.29	**P, sd:**	**0.091**
0.13		Alpha (**A**) =	**0.000**	0.00		
2.57		Beta (**B**)=	0.120	0.17	L, count:	14
		LogL16 (**L**) =	2.761	2.526		
		Vx (**V**)=	0.8680		**L, sd:**	**0.051**

											LogPcalc	LogPobs		
											1.335	1.288		
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)	2.921	2.921	2.830	0.008	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.251	-0.251	-0.254	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	2.534	2.534	2.576	0.002
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.215	-0.215	-0.254	0.001
Ind Eng Chem Proc	SQ	0.703	0.000	0.299	0.000	0.000	1.981	0.000	RI/100	SQ	6.253	6.253	6.296	0.002
Ind Eng Chem Proc	SQ	0.721	0.000	0.666	0.000	-1.095	1.987	0.000	RI/100	SQ	6.255	6.255	6.287	0.001
J High Res Chroma	SE-30 (80C)	0.739	0.000	0.489	1.168	1.009	1.954	0.000	RI/100	SE-30 (80C)	6.387	6.387	6.360	0.001
J High Res Chroma	SE-30 (130C)	0.761	0.339	0.466	1.711	0.000	1.973	0.000	RI/100	SE-30 (130C)	6.468	6.468	6.340	0.016
J of Gas Chromato	SE-30	0.849	0.000	1.272	0.000	-1.744	1.967	0.000	RI/100	SE-30	6.414	6.414	6.420	0.000
J of Gas Chromato	CW-20M (130C)	0.839	0.000	5.616	0.000	0.000	1.961	0.000	RI/100	CW-20M (130C)	7.769	7.769	7.770	0.000
J of Gas Chromato	CW-20M (70C)	0.843	0.000	4.452	0.000	0.000	1.958	0.000	RI/100	CW-20M (70C)	7.451	7.451	7.460	0.000
J of Gas Chromato	TCEP (130C)	0.865	3.693	5.354	0.000	5.197	1.951	0.000	RI/100	TCEP (130C)	9.783	9.783	9.720	0.004
J of Gas Chromato	SQ (27C)	0.879	-0.282	0.527	0.000	0.000	1.922	0.000	RI/100	SQ (27C)	6.216	6.216	6.279	0.004
J of Gas Chromato	SQ (49C)	0.852	-0.269	0.567	0.000	0.000	1.938	0.000	RI/100	SQ (49C)	6.249	6.249	6.288	0.002
J of Gas Chromato	SQ (67C)	0.829	-0.189	0.561	0.000	0.000	1.947	0.000	RI/100	SQ (67C)	6.281	6.281	6.305	0.001
J of Gas Chromato	SQ (86C)	0.773	0.000	0.461	0.000	0.000	1.967	0.000	RI/100	SQ (86C)	6.328	6.328	6.307	0.000