SMILES	C(\C=C\C=C\C=O)CCCC			C_w=	
Compound No.				C_g=	
Compound Name	**(E,E)-2,4-Decadienal**			**log Kw=**	
Molecular Formula	C10H16O			P + L, count:	17
Molecular weight	152.2334	**WS (mg/L)=**			
CAS No	25152-84-5	**VP (mm Hg)=**		**P+L, sd:**	**0.083**
S-A/n20 =	1.515				
E =	0.791			Weight:	1.00
P* **ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
3.270		3.55	3.18	**P+L, sd(W):**	**0.083**

UNIX	**SMART**					
0.54		logKw	3.013	PA	P, count:	2
0.83		R (**E**)=	**0.791**	0.54		
0.00		Pi (**S**)=	0.900	0.95	**P, sd:**	**0.035**
0.47		Alpha (**A**) =	**0.000**	0.00		
5.28		Beta (**B**)=	0.520	0.47	L, count:	15
		LogL16 (**L**) =	5.823	5.533		
		Vx (**V**)=	1.4473		**L, sd:**	**0.088**

												LogPcalc	LogPobs		
												3.160	3.141		
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)	3.305	3.305	3.270	0.001	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.016	3.016	3.013	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	6.181	6.181	6.283	0.010	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.111	3.111	3.013	0.010	
Flav Frag J (2000)	HP5-MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP5-MS	13.231	13.231	13.130	0.010	
Flav Frag J (1999)	HP-1	0.309	-0.579	1.155	1.227	0.000	2.059	0.000	RI/100	HP-1	12.880	12.880	12.840	0.002	
JAFC (2005) 53(8)	DB-5MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB-5MS	13.227	13.227	13.250	0.001	
JAFC (2002) 50(2)	DB-Wax	-0.659	0.000	6.957	10.472	0.000	2.129	0.000	RI/100	DB-Wax	17.999	17.999	17.930	0.005	
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	12.859	12.859	12.840	0.000	
JAFC (1998) 46(2)	HP-Innowax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	HP-Innowax	18.283	na		na	17.780
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	13.259	13.259	13.320	0.004	
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	12.853	12.853	12.890	0.001	
JAFC (2005) 53(5)	Supelcowax-10	-0.484	0.000	7.638	10.527	-2.135	2.132	0.000	RI/100	Supelcowax-10	17.695	17.695	17.840	0.021	
Final Report 2003	DB-5	1.154	0.000	0.000	0.000	1.423	1.922	0.000	RI/100	DB-5	13.086	13.086	13.150	0.004	
JCA (2000) 905 23	CPSil-8CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CPSil-8CB	13.299	13.299	13.270	0.001	
JAFC (2001) 49(3)	1345-1352	0.782	-0.451	1.312	0.808	0.000	1.975	0.000	RI/100		13.106	13.106	13.180	0.005	
JAFC (1991) 39(11	DB-Wax	0.465	-1.373	4.806	1.418	-4.049	2.009	0.000	RI/100	DB-Wax	13.297	13.297	13.170	0.016	
JAFC (2003) 51(5)	DB-5	0.707	0.000	1.225	1.325	0.000	1.972	0.000	RI/100	DB-5	13.292	13.292	13.160	0.018	
"Quant Anal Flav F	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	18.299	na		na	19.380
"Quant Anal Flav F	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	13.422	na		na	13.100