SMILES	C(/CC)=C/CC\C=C\C=O			C_w=	
Compound No.	5453			C_g=	
Compound Name	**(E,Z)-2,6-nonadienal**			**log Kw=**	
Molecular Formula	C9H14O			P + L, count:	15
Molecular weight	138.2100	**WS (mg/L)=**			
CAS No	557-48-2	**/P (mm Hg)=**		**P+L, sd:**	**0.059**
S-A/n20 =	1.474				
E =	0.497			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	2.680		3.07	2.60	**P+L, sd(W):**	**0.059**

UNIX	**SMART**			**PA**		
		logKw	2.688		P, count:	3
0.54		R (**E**)=	**0.497**	**0.54**		
0.83		Pi (**S**)=	0.810	**0.95**	**P, sd:**	**0.078**
0.00		Alpha (**A**) =	**0.000**	**0.00**		
0.47		Beta (**B**)=	0.510	**0.47**	L, count:	12
4.78		LogL16 (**L**) =	5.008	**5.038**		
		Vx (**V**)=	**1.3064**		**L, sd:**	**0.057**

											LogPcalc	LogPobs	
											2.613	2.563	
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)	2.732	2.732	2.680	0.003
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.417	2.417	2.320	0.009
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.691	2.691	2.688	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	5.403	5.403	5.368	0.001	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	5.008	5.008	5.008	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.748	2.748	2.688	0.004	
JAFC (2003) 51(7)	DB-Wax	0.657	0.000	6.952	10.389	-1.377	1.979	0.000	RI/100	DB-Wax	15.497	na		na	15.840
Final Report March	DB-5	1.154	0.000	0.000	0.000	1.423	1.922	0.000	RI/100	DB-5	11.505	11.505	11.500	0.000	
JAFC (2001) 49(3)	1345-1352	0.782	-0.451	1.312	0.808	0.000	1.975	0.000	RI/100		11.512	11.512	11.550	0.001	
JAFC (2005) 53(8)	DB-5MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB-5MS	11.641	11.641	11.540	0.010	
JAFC (2002) 50(2)	DB-Wax	-0.659	0.000	6.957	10.472	0.000	2.129	0.000	RI/100	DB-Wax	15.638	15.638	15.680	0.002	
JAFC (2001) 49(6)	DB-Wax	-2.488	0.000	8.261	11.077	2.463	2.106	0.000	RI/100	DB-Wax	16.007	16.007	15.990	0.000	
JAFC (2000) 48(2)	DB-Wax	-1.307	0.523	9.055	10.206	0.000	1.977	0.000	RI/100	DB-Wax	16.188	na		na	15.800
JAFC (2000) 48(2)	DB-5	-0.139	-1.242	2.721	2.102	0.000	2.016	0.000	RI/100	DB-5	11.544	11.544	11.560	0.000	
Flav Frag J (2003)	DB-5	0.850	0.000	0.951	1.143	0.000	1.970	0.000	RI/100	DB-5	11.486	11.486	11.580	0.009	
Food Chem (2003)	HP-1	0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100	HP-1	11.261	11.261	11.170	0.008	
JAFC (1983) 31(6)	DB-1	0.624	0.000	0.548	0.545	0.404	1.991	0.000	RI/100	DB-1	11.245	11.245	11.230	0.000	