SMILES	C(=C/CCCC)\C=C\C=O			C_w=	
Compound No.	5452			C_g=	
Compound Name	**(E, E)-2,4-Nonadienal**			**log Kw=**	
Molecular Formula	C9H14O			P + L, count:	11
Molecular weight	138.2100	**WS (mg/L)=**			
CAS No	5910-87-2	**VP (mm Hg)=**		**P+L, sd:**	**0.047**
S-A/n20 =	1.521				
E =	0.802			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	2.740		3.07	2.65	**P+L, sd(W):**	**0.047**

UNIX	**SMART**			**PA**		
0.54		logKw	3.091		P, count:	2
0.83		R (**E**)=	**0.802**	**0.54**		
0.00		Pi (**S**)=	0.880	**0.95**	**P, sd:**	**0.055**
0.47		Alpha (**A**) =	**0.000**	**0.00**		
4.78		Beta (**B**)=	0.520	**0.47**	L, count:	9
		LogL16 (**L**) =	5.338	**5.038**		
		Vx (**V**)=	**1.3064**		**L, sd:**	**0.048**

LogPcalc	LogPobs
2.944	2.916

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)	2.795	2.795	2.740	0.003	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.094	3.094	3.091	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	5.751	5.751	5.831	0.006	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.168	3.168	3.091	0.006	
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	12.352	12.352	12.350	0.000	
JAFC (2005) 53(8)	DB5-MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB5-MS	12.233	12.233	12.240	0.000	
JAFC (2002) 50(2)	DB-Wax	-0.659	0.000	6.957	10.472	0.000	2.129	0.000	RI/100	DB-Wax	16.829	16.829	16.810	0.000	
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	11.844	11.844	11.800	0.002	
JAFC (1998) 46(2)	Innowax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	Innowax	17.134	na		na	16.800
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	11.851	11.851	11.870	0.000	
JAFC (2001) 49(3)	1345-1352	0.782	-0.451	1.312	0.808	0.000	1.975	0.000	RI/100		12.118	12.118	12.160	0.002	
Final Report March 2003		1.154	0.000	0.000	0.000	1.423	1.922	0.000	RI/100	DB-5	12.155	12.155	12.110	0.002	