SMILES	C(/CC)=C/CC=O			C_w=	
Compound No.				C_g=	
Compound Name	**(Z)-3-hexenal**			**log Kw=**	
Molecular Formula	C6H10O			P + L, count:	13
Molecular weight	98.1400	**WS (mg/L)=**			
CAS No	6789-80-6	**VP (mm Hg)=**		**P+L, sd:**	**0.077**
S-A/n20 =	1.440				
E =	0.344			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.608	1.608	1.33	1.73	**P+L, sd(W):**	**0.077**

UNIX	**SMART**			**PA**		
0.41		logKw	2.121		P, count:	3
0.73		R (**E**)=	**0.344**	0.39		
0.00		Pi (**S**)=	0.680	0.84	**P, sd:**	**0.085**
0.45		Alpha (**A**) =	**0.000**	0.00		
3.34		Beta (**B**)=	0.420	0.39	L, count:	10
		LogL16 (**L**) =	3.296	3.563		
		Vx (**V**)=	0.9267		**L, sd:**	**0.080**

LogPcalc	LogPobs
1.697	1.635

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)	1.646	1.646	1.608	0.001	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.280	1.280	1.175	0.011	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.166	2.166	2.121	0.002	
											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	3.713	3.713	3.729	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.296	3.296	3.296	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.197	2.197	2.121	0.006	
JAFC (2003) 51(4)	DB-5	1.389	-0.343	1.997	1.784	-1.769	1.910	0.000	RI/100	DB-5	8.181	na		na	7.950
JCA (2003) 998 20	DB-5	0.527	0.000	1.312	0.772	0.000	2.012	0.000	RI/100	DB-5	8.050	8.050	7.950	0.010	
JAFC (1992) 40(5)	DB-1	1.283	-0.242	0.000	0.000	0.000	2.009	0.000	RI/100	DB-1	7.821	7.821	7.690	0.017	
Phytochemistry (19	SF-96	0.096	0.000	1.092	1.639	0.000	2.053	0.000	RI/100	SF-96	7.605	7.605	7.730	0.016	
JAFC (1990) 38(1)	DB-1	-0.171	-0.960	1.669	1.754	-0.444	2.164	0.000	RI/100	DB-1	7.579	7.579	7.650	0.005	
JAFC (2002) 50(4)	DB-5	0.498	0.000	1.245	1.671	0.000	2.005	0.000	RI/100	DB-5	7.952	7.952	7.970	0.000	
JAFC (2002) 50(4)	DB-Wax	0.902	1.137	7.611	15.757	-3.781	2.000	0.000	RI/100	DB-Wax	11.472	11.472	11.470	0.000	
JAFC (1976) 24(6)	OV-1	0.605	-0.378	1.109	1.025	0.000	2.005	0.000	RI/100	OV-1	7.837	7.837	7.780	0.003	