SMILES	C\C(=C\C=C\C(C)=O)C			C_w=	
Compound No.	5789			C_g=	
Compound Name	**6-Methyl-3,5-heptadiene-2-one**			**log Kw=**	
Molecular Formula	C8H12O			P + L, count:	9
Molecular weight	124.1800	**WS (mg/L)=**			
CAS No	1604-28-0	**VP (mm Hg)=**		**P+L, sd:**	**0.072**
S-A/n20 =	1.536				
E =	0.859			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.549		1.78	1.66	**P+L, sd(W):**	**0.072**

UNIX	**SMART**			**PA**		
0.56		logKw	4.132		P, count:	2
0.78		R (**E**)=	**0.859**	**0.50**		
0.00		Pi (**S**)=	0.790	**0.83**	**P, sd:**	**0.039**
0.47		Alpha (**A**) =	**0.000**	**0.00**		
4.23		Beta (**B**)=	0.750	**0.49**	L, count:	7
		LogL16 (**L**) =	4.906	**4.273**		
		Vx (**V**)=	1.1655		**L, sd:**	**0.082**

											LogPcalc	LogPobs		
											2.861	2.841		
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)	1.588	1.588	1.549	0.002	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.133	4.133	4.132	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	5.645	5.645	5.681	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.168	4.168	4.132	0.001	
Flav Frag J (2001)	Optima 1	-0.033	-0.625	1.546	1.513	0.000	2.083	0.000	RI/100	Optima 1	10.871	10.871	10.840	0.001	
JAFC (1990) 38(1)	DB-1	-0.171	-0.960	1.669	1.754	-0.444	2.164	0.000	RI/100	DB-1	10.607	10.607	10.740	0.018	
Flav Frag J (2000)	Optima 1	0.414	-0.447	1.217	1.678	0.000	2.034	0.000	RI/100	Optima 1	10.971	10.971	10.850	0.015	
Forest Polar and N	DB-1	0.569	-0.446	1.091	1.756	-0.349	2.025	0.000	RI/100	DB-1	10.721	10.721	10.764	0.002	
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	10.812	10.812	10.760	0.003	