SMILES	C1\C=C(/C(C1)=O)C			C_w=	
Compound No.	5797			C_g=	
Compound Name	**2-Methyl-2-cyclopentenone**			**log Kw=**	
Molecular Formula	C6H8O			P + L, count:	14
Molecular weight	96.1300	**WS (mg/L)=**			
CAS No	1120-73-6	**VP (mm Hg)=**		**P+L, sd:**	**0.067**
S-A/n20 =	1.479				
E =	0.529			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	0.491	0.491	0.79	0.54	**P+L, sd(W):**	**0.067**

UNIX	SMART			PA		
		logKw	3.965		P, count:	3
0.63		R (**E**)=	**0.529**	0.56		
0.83		Pi (**S**)=	0.940	0.81	**P, sd:**	**0.109**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.43		Beta (**B**)=	0.600	0.40	L, count:	11
3.65		LogL16 (**L**) =	3.720	3.580		
		Vx (**V**)=	0.8181		**L, sd:**	**0.059**

LogPcalc	LogPobs
1.322	1.404

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)	0.439	0.439	0.491	0.003	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.375	-0.375	-0.246	0.017	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.901	3.901	3.965	0.004	

											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	4.518	4.518	4.456	0.004
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.720	3.720	3.720	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.838	3.838	3.965	0.016
Atmos Chem Phys	DB-5	0.565	-0.099	1.062	0.960	0.000	2.024	0.000	RI/100	DB-5	9.040	9.040	9.076	0.001
Meat Sci (1996) 44	DB-5	0.493	-0.430	1.327	1.408	0.000	2.048	0.000	RI/100	DB-5	9.131	9.131	9.150	0.000
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	9.247	9.247	9.220	0.001
JAFC (2001) 49(9)	BPX-5	1.344	0.000	0.769	0.978	0.330	1.850	0.000	RI/100	BPX-5	9.146	9.146	9.200	0.003
Food Chem (2004)	CP-Sil-8CB	0.532	-0.473	1.552	1.340	-0.344	2.030	0.000	RI/100	CP-Sil-8CB	9.085	9.085	9.150	0.004
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	9.246	9.246	9.220	0.001
JAFC (1999) 47(12	CP-Wax-52CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CP-Wax-52CB	13.603	13.603	13.550	0.003
JAFC (1999) 47(12	CP-Sil-8CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CP-Sil-8CB	8.968	8.968	9.010	0.002