SMILES	C1C(/C=C\C1)=O			C_w=	
Compound No.	5799			C_g=	
Compound Name	**Cyclopentenone**			**log Kw=**	
Molecular Formula	C5H6O			P + L, count:	8
Molecular weight	82.1000	**WS (mg/L)=**			
CAS No	930-30-3	**VP (mm Hg)=**		**P+L, sd:**	**0.068**
S-A/n20 =	1.481				
E =	**0.535**			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	-0.030	-0.028	0.40	-0.05	**P+L, sd(W):**	**0.068**

UNIX	SMART			PA		
0.63		logKw	4.149		P, count:	2
0.85		R (**E**)=	**0.535**	0.58		
0.00		Pi (**S**)=	1.070	0.86	**P, sd:**	**0.066**
0.43		Alpha (**A**) =	**0.000**	0.00		
3.17		Beta (**B**)=	0.560	0.38	L, count:	6
		LogL16 (**L**) =	3.241	3.221		
		Vx (**V**)=	0.6772		**L, sd:**	**0.075**

LogPcalc	LogPobs
2.035	2.059

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)	-0.094	-0.094	-0.030	0.004	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.165	4.165	4.149	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	4.143	4.143	4.119	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.109	4.109	4.149	0.002	
JAFC (2002) 50(6)	HP-5	0.480	-0.537	1.445	1.169	0.000	2.030	0.000	RI/100	HP-5	8.319	na		na	8.020
JAFC (1998) 46(6)	DB-1	1.589	0.000	0.742	0.824	0.000	1.744	0.000	RI/100	DB-1	8.036	8.036	7.990	0.002	
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	7.994	7.994	7.930	0.004	
Atmos Chem Phys	DB-5	0.565	-0.099	1.062	0.960	0.000	2.024	0.000	RI/100	DB-5	8.209	8.209	8.349	0.020	
JAFC (1972) 20(5)	CW-20M	-6.962	1.301	6.179	9.208	0.000	2.152	0.000	RI/100	CW-20M	7.321	7.321	7.300	0.000	