SMILES	C1(/C)=C\C(CC1)=O			C_w=	
Compound No.	5777			C_g=	
Compound Name	**3-Methyl-2-cyclopentenone**			**log Kw=**	
Molecular Formula	C6H8O			P + L, count:	10
Molecular weight	96.1300	**WS (mg/L)=**			
CAS No	2758-18-1	**VP (mm Hg)=**		**P+L, sd:**	**0.059**
S-A/n20 =	1.488				
E =	0.567			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	0.491	0.491	0.79	0.54	**P+L, sd(W):**	**0.059**

UNIX	SMART			PA		
0.63		logKw	4.146		P, count:	3
0.83		R (**E**)=	**0.567**	0.56		
0.00		Pi (**S**)=	1.250	0.81	**P, sd:**	**0.050**
0.43		Alpha (**A**) =	**0.000**	0.00		
3.65		Beta (**B**)=	0.490	0.40	L, count:	7
		LogL16 (**L**) =	3.773	3.580		
		Vx (**V**)=	0.8181		**L, sd:**	**0.066**

LogPcalc	LogPobs
1.460	1.421

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)	0.514	0.514	0.491	0.001	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.315	-0.315	-0.373	0.003	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.181	4.181	4.146	0.001	

											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	4.627	4.627	4.637	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.773	3.773	3.773	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.179	4.179	4.146	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	9.634	9.634	9.730	0.009
JAFC (1996) 44(3)	Db-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	Db-1	9.322	9.322	9.230	0.008
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	9.694	9.694	9.730	0.001
JAFC (1990) 38(11	DB-5	1.496	0.518	0.000	1.405	0.982	2.035	0.000	RI/100	DB-5	9.948	9.948	9.870	0.006