SMILES	CC(CC(C)(O)C)=O			C_w=	8.609
Compund No.	8474			C_g=	########
Compund Name	**4-Hydroxy-4-methyl-2-pentanone**			**log Kw=**	4.971
Molecular Formula	C6H12O2			P + L, count:	9
Molecular weight	116.1583	**WS=**	1.00E+06		
CAS No	123-42-2	**VP=**	1.71	**P+L, sd:**	**0.066**
S-A/n20 =	1.423				
E =	**0.232**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
-	-0.05	-0.05	0.35	-0.09	**P+L, sd(W):**	**0.066**

UNIX	**SMART**			**PA**		
0.43	0.223	logKw	**4.971**		P, count:	3
0.85	0.93	R (**E**)=	**0.232**	**0.24**		
0.35	0.31	Pi (**S**)=	0.620	**0.65**	**P, sd:**	**0.031**
0.78	0.95	Alpha (**A**) =	0.060	**0.31**		
3.82	3.940	Beta (**B**)=	1.020	**0.93**	L, count:	6
	1.0284	LogL16 (**L**) =	3.551	**3.784**		
		Vx (**V**)=	**1.0284**		**L, sd:**	**0.082**

											LogPcalc	LogPobs		
											1.190	1.167		
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)	-0.040	-0.040	-0.050	0.000	CLOGP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-1.383	-1.383	-1.420	0.001	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.993	4.993	4.971	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	4.958	4.958	4.921	0.001
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	5.008	5.008	4.971	0.001
Atmos. Chem. Ph	DB-5	0.565	-0.099	1.062	0.960	0.000	2.024	0.000	RI/100	DB-5	8.446	8.446	8.413	0.001
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	8.002	8.002	8.140	0.019
Phytochemistry (1	DB-5	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100	DB-5	8.502	8.502	8.400	0.010
JAFC (1998) 46(12	DB-5	0.679	0.000	1.070	1.587	0.000	1.994	0.000	RI/100	DB-5	8.519	8.519	8.510	0.000