SMILES	C(C(C=C)=O)C			C_w=	
Compound No.	5773			C_g=	
Compound Name	**1-Penten-3-one**			**log Kw=**	
Molecular Formula	C5H8O			P + L, count:	12
Molecular weight	84.1200	**WS (mg/L)=**			
CAS No	1629-58-9	**VP (mm Hg)=**		**P+L, sd:**	**0.085**
S-A/n20 =	1.419				
E =	0.285			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	0.516		0.76	0.57	**P+L, sd(W):**	**0.085**

UNIX	SMART			PA		
		logKw	2.945		P, count:	3
0.41		R (**E**)=	**0.285**	0.34		
0.64		Pi (**S**)=	0.720	0.74	**P, sd:**	**0.091**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.45		Beta (**B**)=	0.550	0.39	L, count:	9
2.77		LogL16 (**L**) =	2.761	2.881		
		Vx (**V**)=	0.7858		**L, sd:**	**0.088**

LogPcalc	LogPobs
1.162	1.092

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)	0.583	0.583	0.516	0.005	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.082	-0.082	-0.183	0.010	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.985	2.985	2.945	0.002	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	logL(calc)	logL(calc)	logL(obs)	(Po-Pc)^2	
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	3.468	3.468	3.461	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	2.761	2.761	2.761	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.998	2.998	2.945	0.003	
JAFC (2003) 51(22	SW	0.282	0.000	6.961	10.552	-1.721	2.055	0.000	RI/100	SW	10.022	10.022	10.130	0.012	
JAFC (2003) 51(22	SPB-1	0.232	-0.398	1.027	1.098	0.000	2.087	0.000	RI/100	SPB-1	6.621	6.621	6.620	0.000	
JAFC (2002) 50(19	HP-5	0.538	-0.519	1.419	0.822	0.000	2.029	0.000	RI/100	HP-5	7.014	na		na	6.800
JAFC (2002) 50(22	HP-5MS	0.691	-0.352	1.227	1.125	0.000	1.989	0.000	RI/100	HP-5MS	6.966	6.966	6.840	0.016	
JAFC (1995) 43(7)	DB-1	0.313	0.000	0.637	0.865	0.241	2.058	0.000	RI/100	DB-1	6.587	6.587	6.600	0.000	
JAFC (1989) 37(2)	DB-Wax	-0.435	1.072	6.781	9.721	0.000	2.013	0.000	RI/100	DB-Wax	10.311	10.311	10.160	0.023	
JAFC (1990) 38(1)	DB-1	-0.171	-0.960	1.669	1.754	-0.444	2.164	0.000	RI/100	DB-1	6.488	6.488	6.580	0.008	