SMILES	C1(OCCC1)=O				
Compund No.	5971				
Compund Name	**g-Butyrolactone**				
Molecular Formula	C4H6O2			P + L, count:	10
Molecular weight	86.0890				
CAS No	96-48-0			**P+L, sd:**	**0.071**
S-A/n20 =	1.436				
E =	**0.387**			Weight:	1.00
		MD	**PA**	**ACD**	
ClogP		-0.860	-0.41	-0.76	**P+L, sd(W):** **0.071**

UNIX	**SMART**			**PA**		
		logKw	5.043		P, count:	2
0.50	0.366	R (**E**)=	**0.387**	0.37		
1.30	1.27	Pi (**S**)=	1.38	0.89	**P, sd:**	**0.117**
0.00	0.00	Alpha (**A**) =	**0.00**	0.00		
0.53	0.58	Beta (**B**)=	0.59	0.53	L, count:	8
3.50	2.941	LogL16 (**L**) =	3.321	2.931		
	0.6380	Vx (**V**)=	0.6380		**L, sd:**	**0.068**

LogPcalc	LogPobs
2.146	2.201

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)	-0.757	-0.757	-0.640	0.014
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.049	5.049	5.043	0.000

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	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	4.474	4.474	4.403	0.005
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.965	4.965	5.043	0.006
JAFC (1989) 37(3)	SE-54	0.711	-0.377	1.042	1.019	0.219	1.985	0.000	RI/100	SE-54	8.725	na		na
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	8.613	8.613	8.570	0.002
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	8.429	8.429	8.540	0.012
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	8.499	8.499	8.560	0.004
JAFC (1998) 46 51	DB-5	0.679	0.000	1.070	1.587	0.000	1.994	0.000	RI/100	DB-5	8.778	na		na
JAFC (2001) 49(3)	HP-WAX	-1.665	1.338	7.944	11.828	-0.724	2.220	0.000	RI/100	HP-WAX	16.762	16.762	16.730	0.001
Food Chem (1999) 64 3-11		0.045	-0.609	1.664	1.596	-0.555	2.067	0.000	RI/100		8.643	8.643	8.600	0.002
Food Res Int (2001	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	9.159	9.159	9.150	0.000