SMILES	C1CCCOC1=O
Compund No.	5974
Compund Name	**d-Pentanolactone**
Molecular Formula	C5H8O2
Molecular weight	100.1158
CAS No	542-28-9
S-A/n20 =	1.457
E =	**0.441**

P + L, count:	10
P+L, sd:	**0.111**
Weight:	1.00
P+L, sd(W):	**0.111**

P*	**ClogP(MD)**	**ClogP(PA)**	**ClogP(ACD)**
-0.350	-0.244	-0.02	-0.24

UNIX	**SMART**			PA		
		logKw	5.447		P, count:	4
0.50	0.445	R (**E**)=	**0.441**	0.445		
1.30	1.54	Pi (**S**)=	1.520	1.54	**P, sd:**	**0.123**
0.00	0.00	Alpha (**A**) =	**0.000**	0.00		
0.53	0.62	Beta (**B**)=	0.630	0.62	L, count:	6
4.00		LogL16 (**L**) =	3.680	4.000		
		Vx (**V**)=	**0.7789**		**L, sd:**	**0.114**

LogPcalc	LogPobs
1.087	1.077

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)	-0.475	-0.475	**-0.350**	0.016
Jamie	Trichloromethane	0.327	0.157	-0.391	-3.191	-3.437	0.000	4.191	P	Trichloromethane	0.901	0.901	**0.950**	0.002
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.508	5.508	5.447	0.004
CYC-1	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577	P	Cyclohexane/Dec 98	-1.586	-1.586	**-1.740**	0.024

											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	4.938	4.938	5.097	0.025
	Chloroform	0.116	-0.467	1.203	0.138	1.432	0.994	0.000	L	CHCl3/Wet/25.8.97	6.299	6.299	6.397	0.010
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	5.510	5.510	5.447	0.004
CYC-1	Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013	0.000	L	Cyclohexane/Dec/98	3.842	3.842	3.707	0.018
JAFC (1984) 32(5) 1011-1015		0.601	-0.257	0.942	1.309	0.000	1.996	0.000	RI/100		9.265	9.265	9.180	0.007
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	9.401	9.401	9.430	0.001

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