SMILES	CC1(C)CC(C)CCC1		C_w= 0.000
Compound No.	718		C_g= 0.000
Compound Name	**1,1,3-Trimethylcyclohexane**		**log Kw=** #DIV/0!
Molecular Formula	C9H18		P + L, count: 12
Molecular weight	126.2400	**WS (mg/L)= 1.770**	
CAS No	3073-66-3	**VP (mm Hg)=**	**P+L, sd: 0.028**
Beil/n20 =	1.430		
E =	**0.206**		Weight: 1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	4.910	4.911	3.92	4.91	**P+L, sd(W): 0.028**

UNIX	**SMART**			**PA**	
0.31	0.320	logKw	-1.740		P, count: 2
0.16	0.17	R (**E**)=	**0.206**	0.20	
0.00	0.00	Pi (**S**)=	0.080	0.21	**P, sd: 0.057**
0.15	0.00	Alpha (**A**) =	**0.000**	0.00	
3.97	4.17 (L57)	Beta (**B**)=	0.000	0.09	L, count: 10
		LogL16 (**L**) =	3.856	4.053	
		Vx (**V**)=	1.2681		**L, sd: 0.025**

											LogPcalc	LogPobs		
											1.591	1.585		
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)	4.956	4.956	4.910	0.002	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-1.773	-1.773	-1.740	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	3.168	3.168	3.170	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-1.704	-1.704	-1.740	0.001
JCA (1982) 253 17	OV-101	0.440	-0.641	0.869	0.000	0.994	2.062	0.000	RI/100	OV-101	8.329	8.329	8.304	0.001
J High Res Chrom	Petrol-DH	0.579	-0.342	0.755	0.869	0.983	2.014	0.000	RI/100	Petrol-DH	8.336	8.336	8.328	0.000
J Sep Sci (2001) 2	OV-101	0.627	-0.271	0.000	0.000	2.356	2.017	0.000	RI/100	OV-101	8.349	8.349	8.355	0.000
Chromatographia (	SQ (50C)	0.649	-0.229	0.624	0.000	-0.495	2.010	0.000	RI/100	SQ (50C)	8.403	8.403	8.404	0.000
Chromatographia (	SQ (70C)	0.627	-0.193	0.698	0.000	-0.740	2.024	0.000	RI/100	SQ (70C)	8.448	8.448	8.460	0.000
Chromatographia (	Citroflex (50C)	0.720	-0.707	3.164	0.000	1.627	1.997	0.000	RI/100	Citroflex (50C)	8.529	8.529	8.502	0.001
Chromatographia (	Citroflex (70C)	0.688	-0.657	3.187	0.000	1.378	2.013	0.000	RI/100	Citroflex (70C)	8.570	8.570	8.559	0.000
California EPA Pro	Supelco-Petrocol-DH1	0.712	0.000	0.434	1.113	0.484	1.995	0.000	RI/100	Supelco-Petrocol-DH100	8.440	8.440	8.490	0.002