SMILES	C1(CCCCC1)C2CCCCC2			C_w=	0.000
Compound No.	890			C_g=	0.000
Compound Name	**Dicyclohexyl**			**log Kw=**	#NUM!
Molecular Formula	C12H22			P + L, count:	9
Molecular weight	166.3000	**WS (mg/L)=**			
CAS No	92-51-3	**VP (mm Hg)=**	**0.108**	**P+L, sd:**	**0.086**
S-A/n20 =	1.478				
E =	**0.523**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	5.904	5.904	5.02	5.94	**P+L, sd(W):**	**0.086**

UNIX	**SMART**			**PA**		
		logKw	-0.655		P, count:	2
0.53	0.531	R (**E**)=	**0.523**	0.43		
0.35	0.30	Pi (**S**)=	0.450	0.36	**P, sd:**	**0.123**
0.00	0.00	Alpha (**A**) =	**0.000**	0.00		
0.10	0.00	Beta (**B**)=	0.040	0.07	L, count:	7
6.01		LogL16 (**L**) =	6.047	6.044		
		Vx (**V**)=	1.5822		**L, sd:**	**0.086**

LogPcalc	LogPobs
2.539	2.624

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)	5.804	5.804	5.904	0.010	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.726	-0.726	-0.655	0.005	

											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	5.367	5.367	5.249	0.014
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.702	-0.702	-0.655	0.002
Fuel (1995) 74(10)	Rtx-50 (2C)	0.434	1.793	0.628	1.953	1.722	2.014	0.000	RI/100	Rtx-50 (2C)	13.902	13.902	13.775	0.016
Fuel (1995) 74(10)	Rtx-50 (6C)	0.424	2.339	0.000	2.021	2.124	2.015	0.000	RI/100	Rtx-50 (6C)	13.917	13.917	13.974	0.003
Fuel (1995) 74(10)	DB-5 (2C)	0.461	1.130	-0.691	1.324	0.926	2.010	0.000	RI/100	DB-5 (2C)	12.932	12.932	12.931	0.000
Fuel (1995) 74(10)	DB-5 (6C)	0.452	1.239	-0.645	1.203	0.818	2.011	0.000	RI/100	DB-5 (6C)	13.003	13.003	13.078	0.006
J High Res Chroma	SE-30	0.761	0.339	0.466	1.711	0.000	1.973	0.000	RI/100	SE-30	13.078	13.078	13.130	0.003