SMILES	C(CCCCCC)CCC(C)C			C_w=	0.000
Compound No.	310			C_g=	0.000
Compound Name	**2-Methylundecane**			**log Kw=**	#DIV/0!
Molecular Formula	C12H26			P + L, count:	10
Molecular weight	170.3300	**WS (mg/L)=**			
CAS No	7045-71-8	**VP (mm Hg)=**		**P+L, sd:**	**0.073**
Beil/n20 =	1.420				
E =	**-0.017**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	6.912		5.96	6.95	**P+L, sd(W):**	**0.073**

UNIX	-2.449	logKw	-2.483	PA	P, count:	2
0.13	**-0.017**	R (**E**)=	**-0.017**	0.00		
0.09	0.000	Pi (**S**)=	0.000	0.20	**P, sd:**	**0.090**
0.00	**0.000**	Alpha (**A**) =	**0.000**	0.00		
0.11	0.010	Beta (**B**)=	**0.000**	0.09	L, count:	8
5.52	5.434	LogL16 (**L**) =	5.448	5.582		
	1.7994	Vx (**V**)=	1.7994		**L, sd:**	**0.075**

LogPcalc	LogPobs
2.187	2.215

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)	6.941	6.941	6.912	0.001	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-2.567	-2.567	-2.483	0.007	

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	4.477	4.477	4.429	0.002
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-2.445	-2.445	-2.483	0.001
J Anal Chem USSR (2002) 57(6) 544-551		0.711	-2.712	-11.286	0.000	18.609	1.983	0.000	RI/100		11.561	11.561	11.630	0.005
Atmos. Chem. Phy:	DB-5	0.565	-0.099	1.062	0.960	0.000	2.024	0.000	RI/100	DB-5	11.594	11.594	11.651	0.003
J Chromatog (1982	OV-101	0.440	-0.641	0.869	0.000	0.994	2.062	0.000	RI/100	OV-101	11.685	11.685	11.649	0.001
J High Res Chromá	Methyl silicone	0.443	-1.058	1.625	0.000	0.000	2.069	0.000	RI/100	Methyl silicone	11.733	11.733	11.653	0.006
J High Res Chromá	phenyl-methyl silicone	0.401	-0.832	1.685	0.000	0.000	2.078	0.000	RI/100	phenyl-methyl silicone	11.737	11.737	11.644	0.009
JAFC (1989) 37(3)	SE-54	0.711	-0.377	1.042	1.019	0.219	1.985	0.000	RI/100	SE-54	11.532	11.532	11.640	0.012