SMILES	C(C(C=C)(C)C)C		C_w= 0.000
Compound No.	1037		C_g= 0.006
Compound Name	**3,3-Dimethyl-1-pentene**		**log Kw=** #NUM!
Molecular Formula	C7H14		P + L, count: 13
Molecular weight	98.1900	**WS (mg/L)=**	
CAS No	3404-73-7	**VP (mm Hg)= 104**	**P+L, sd: 0.059**
Beil/n20 =	1.398		
E =	**0.088**		Weight: 1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	3.653	3.653	3.29	3.60	**P+L, sd(W): 0.059**

UNIX	**SMART**			**PA**	
0.25	0.088	logKw	-1.213		P, count: 2
0.09		R (**E**)=	**0.088**	0.11	
0.00	0.00	Pi (**S**)=	0.060	0.19	**P, sd: 0.087**
0.17		Alpha (**A**) =	**0.000**	0.00	
2.74	2.806	Beta (**B**)=	0.100	0.13	L, count: 11
		LogL16 (**L**) =	2.790	2.830	
		Vx (**V**)=	1.0519		**L, sd: 0.059**

LogPcalc	LogPobs
1.260	1.220

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)	3.740	3.740	3.653	0.008	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-1.220	-1.220	-1.213	0.000	

											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	2.382	2.382	2.440	0.003	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-1.147	-1.147	-1.213	0.004	
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	6.353	6.353	6.210	0.021	
J Gas Chrom. (196	SQ (27C)	0.879	-0.282	0.527	0.000	0.000	1.922	0.000	RI/100	SQ (27C)	6.249	6.249	6.239	0.000	
J Gas Chrom. (196	SQ (49C)	0.852	-0.269	0.567	0.000	0.000	1.938	0.000	RI/100	SQ (49C)	6.270	6.270	6.270	0.000	
J Gas Chrom. (196	SQ (67C)	0.829	-0.189	0.561	0.000	0.000	1.947	0.000	RI/100	SQ (67C)	6.279	6.279	6.295	0.000	
J Gas Chrom. (196	SQ (86C)	0.773	0.000	0.461	0.000	0.000	1.967	0.000	RI/100	SQ (86C)	6.289	6.289	6.315	0.001	
Chromatographia (:	SQ (50C)	0.649	-0.229	0.624	0.000	-0.495	2.010	0.000	RI/100	SQ (50C)	6.225	6.225	6.262	0.001	
Chromatographia (:	SQ (70C)	0.627	-0.193	0.698	0.000	-0.740	2.024	0.000	RI/100	SQ (70C)	6.226	6.226	6.285	0.004	
Chromatographia (:	Citroflex (50C)	0.720	-0.707	3.164	0.000	1.627	1.997	0.000	RI/100	Citroflex (50C)	6.583	6.583	6.560	0.001	
Chromatographia (:	Citroflex (70C)	0.688	-0.657	3.187	0.000	1.378	2.013	0.000	RI/100	Citroflex (70C)	6.576	6.576	6.581	0.000	