SMILES	C(=C(\C)C)\CCC			C_w=	
Compound No.	1061			C_g=	
Compound Name	**2-Methyl-2-hexene**			**log Kw=**	
Molecular Formula	C7H14			P + L, count:	12
Molecular weight	98.1900	**WS (mg/L)=**			
CAS No	2738-19-4	**VP (mm Hg)=**		**P+L, sd:**	**0.020**
Beil/n20 =	1.410				
E =	**0.153**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	3.783	3.783	3.31	3.98	**P+L, sd(W):**	**0.020**

UNIX	**SMART**			**PA**		
0.29		logKw	-1.132		P, count:	2
0.21		R (**E**)=	**0.153**	0.13		
0.00		Pi (**S**)=	0.090	0.24	**P, sd:**	**0.023**
0.11		Alpha (**A**) =	**0.000**	0.00		
3.17		Beta (**B**)=	0.090	0.12	L, count:	10
		LogL16 (**L**) =	3.120	3.081		
		Vx (**V**)=	1.0519		**L, sd:**	**0.020**

LogPcalc	LogPobs
1.312	1.326

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)	3.780	3.780	3.783	0.000	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-1.155	-1.155	-1.132	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	2.672	2.672	2.651	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-1.130	-1.130	-1.132	0.000	
J. Gas Chrom. (19	Squalene (27C)	0.879	-0.282	0.527	0.000	0.000	1.922	0.000	RI/100	Squalene (27C)	6.880	6.880	6.919	0.002	
J. Gas Chrom. (19	Squalene (49C)	0.852	-0.269	0.567	0.000	0.000	1.938	0.000	RI/100	Squalene (49C)	6.908	6.908	6.917	0.000	
J. Gas Chrom. (19	Squalene (67C)	0.829	-0.189	0.561	0.000	0.000	1.947	0.000	RI/100	Squalene (67C)	6.925	6.925	6.918	0.000	
J. Gas Chrom. (19	Squalene (86C)	0.773	0.000	0.461	0.000	0.000	1.967	0.000	RI/100	Squalene (86C)	6.952	6.952	6.916	0.001	
Chromatographia (	Squalene (50C)	0.649	-0.229	0.624	0.000	-0.495	2.010	0.000	RI/100	Squalene (50C)	6.897	6.897	6.912	0.000	
Chromatographia (	Squalene (70C)	0.627	-0.193	0.698	0.000	-0.740	2.024	0.000	RI/100	Squalene (70C)	6.909	6.909	6.912	0.000	
Chromatographia (	Citroflex (50C)	0.720	-0.707	3.164	0.000	1.627	1.997	0.000	RI/100	Citroflex (50C)	7.274	7.274	7.272	0.000	
Chromatographia (	Citroflex (70C)	0.688	-0.657	3.187	0.000	1.378	2.013	0.000	RI/100	Citroflex (70C)	7.279	7.279	7.267	0.000	