SMILES	C(=CC)=C			C_w=	
Compound No.	1148			C_g=	
Compound Name	**1,2-Butadiene**			**log Kw=**	
Molecular Formula	C4H6			P + L, count:	14
Molecular weight	54.0904	**WS (mg/L)=**			
CAS No	590-19-2	**VP (mm Hg)=**		**P+L, sd:**	**0.037**
ACD/n20 =	1.376				
E =				Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.902	1.902	1.89	1.97	**P+L, sd(W):**	**0.037**

UNIX	**SMART**			**PA**		
0.31		logKv	-0.265		P, count:	3
0.21		R (**E**)=	0.310	**0.20**		
0.00	0.00	Pi (**S**)=	0.210	**0.30**	**P, sd:**	**0.016**
0.14		Alpha (**A**) =	**0.000**	**0.00**		
1.49		Beta (**B**)=	0.110	**0.12**	L, count:	11
		LogL16 (**L**) =	1.773	**1.540**		
		Vx (**V**)=	0.5862		**L, sd:**	**0.042**

LogPcalc	LogPobs
1.219	1.225

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)	1.896	1.896	1.902	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.017	2.017	2.038	0.000
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.257	-0.257	-0.265	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	1.630	1.630	1.637	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.288	-0.288	-0.265	0.001
Ind Eng Chem Pro	Squalene	0.703	0.000	0.299	0.000	0.000	1.981	0.000	RI/100	Squalene	4.278	4.278	4.285	0.000
Ind Eng Chem Pro	Squalene	0.721	0.000	0.666	0.000	-1.095	1.987	0.000	RI/100	Squalene	4.263	4.263	4.279	0.000
J Gas Chromatog	Squalene	0.879	-0.282	0.527	0.000	0.000	1.922	0.000	RI/100	Squalene	4.310	4.310	4.294	0.000
J Gas Chromatog	Squalene	0.852	-0.269	0.567	0.000	0.000	1.938	0.000	RI/100	Squalene	4.324	4.324	4.304	0.000
J Gas Chromatog	Squalene	0.829	-0.189	0.561	0.000	0.000	1.947	0.000	RI/100	Squalene	4.340	4.340	4.303	0.001
J Gas Chromatog	Squalene	0.773	0.000	0.461	0.000	0.000	1.967	0.000	RI/100	Squalene	4.357	4.357	4.304	0.003
Bull Soc Chim Fr	Squalene	0.888	-1.550	2.169	1.834	0.000	1.915	0.000	RI/100	Squalene	4.258	4.258	4.270	0.000
Bull Soc Chim Fr	Dimethylsulfolane	0.862	1.587	3.804	8.466	1.683	1.940	0.000	RI/100	Dimethylsulfolane	5.778	5.778	5.760	0.000
Procedure for the	SUPELCO Petrocol DH	0.712	0.000	0.434	1.113	0.484	1.995	0.000	RI/100	SUPELCO Petrocol DH-	4.394	4.394	4.500	0.011