SMILES	C=C=C			C_w=	0.000
Compound No.	1140			C_g=	0.000
Compound Name	**1,2-Propadiene**			**log Kw=**	#DIV/0!
Molecular Formula	C3H4			P + L, count:	11
Molecular weight	40.0639	**WS (mg/L)=**			
CAS No	463-49-0	**VP (mm Hg)=**		**P+L, sd:**	**0.021**
ACD/n20 =	1.339				
E =				Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
1.450	1.370	1.370	1.38	1.45	**P+L, sd(W):**	**0.021**

UNIX	**SMART**			**PA**		
0.30	0.330	logKw	-0.365		P, count:	3
		R (**E**)=	0.225	**0.17**		
0.15		Pi (**S**)=	0.277	**0.26**	**P, sd:**	**0.032**
0.00	0.00	Alpha (**A**) =	0.000	**0.00**		
0.14		Beta (**B**)=	0.045	**0.11**	L, count:	8
0.94		LogL16 (**L**) =	1.161	**0.993**		
		Vx (**V**)=	0.4453		**L, sd:**	**0.019**

LogPcalc	LogPobs
0.894	0.870

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)	1.466	1.466	1.450	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.545	1.545	1.526	0.000
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.328	-0.328	-0.365	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	1.059	1.059	1.085	0.001
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.357	-0.357	-0.365	0.000
Bull Soc Chim Fr	Squalene	0.888	-1.550	2.169	1.834	0.000	1.915	0.000	RI/100	Squalene	3.361	3.361	3.360	0.000
Bull Soc Chim Fr	Dimethylsulfolane	0.862	1.587	3.804	8.466	1.683	1.940	0.000	RI/100	Dimethylsulfolane	4.600	4.600	4.620	0.000
J Gas Chromatog	Squalene	0.879	-0.282	0.527	0.000	0.000	1.922	0.000	RI/100	Squalene	3.192	3.192	3.170	0.000
J Gas Chromatog	Squalene	0.852	-0.269	0.567	0.000	0.000	1.938	0.000	RI/100	Squalene	3.198	3.198	3.177	0.000
J Gas Chromatog	Squalene	0.829	-0.189	0.561	0.000	0.000	1.947	0.000	RI/100	Squalene	3.202	3.202	3.189	0.000
J Gas Chromatog	Squalene	0.773	0.000	0.461	0.000	0.000	1.967	0.000	RI/100	Squalene	3.184	3.184	3.198	0.000