SMILES	C(=C(/C=O)C)\C			C_w=	
Compound No.				C_g=	
Compound Name	**trans-2-Methyl-2-butenal**			**log Kw=**	
Molecular Formula	C5H8O			P + L, count:	11
Molecular weight	84.1200	**WS (mg/L)=**			
CAS No	497-03-0	**VP (mm Hg)=**		**P+L, sd:**	**0.072**
S-A/n20 =	1.448				
E =	0.404			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	0.829	0.829	1.08	1.07	**P+L, sd(W):**	**0.072**

UNIX	SMART			PA		
		logKw	2.779		P, count:	3
0.42		R (**E**)=	**0.404**	0.37		
0.70		Pi (**S**)=	0.730	0.78	**P, sd:**	**0.022**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.45		Beta (**B**)=	0.490	0.41	L, count:	8
2.82		LogL16 (**L**) =	3.030	2.933		
		Vx (**V**)=	0.7858		**L, sd:**	**0.085**

LogPcalc	LogPobs
1.303	1.286

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)	0.847	0.847	0.829	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	0.274	0.274	0.252	0.000
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.789	2.789	2.779	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	3.621	3.621	3.608	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.030	3.030	3.030	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.777	2.777	2.779	0.000
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	7.600	7.600	7.550	0.002
JAFC (1989) 37(2)	DB-Wax	-0.435	1.072	6.781	9.721	0.000	2.013	0.000	RI/100	DB-Wax	11.048	11.048	10.900	0.022
JAFC (1990) 38(2)	DB-1	0.228	-0.447	1.253	1.533	-0.451	2.088	0.000	RI/100	DB-1	7.068	7.068	7.150	0.007
JAFC (1990) 38(2)	DB-Wax	-0.548	0.707	6.479	10.014	-0.658	2.192	0.000	RI/100	DB-Wax	10.787	10.787	10.920	0.018
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	7.668	7.668	7.630	0.001