SMILES	CC\C=C(\C=O)C			C_w=	
Compound No.	**5415**			C_g=	
Compound Name	**2-Methylpent-2-en-1-al**			**log Kw=**	
Molecular Formula	C6H10O			P + L, count:	12
Molecular weight	98.1400	**WS (mg/L)=**			
CAS No	623-36-9	**VP (mm Hg)=**		**P+L, sd:**	**0.069**
S-A/n20 =	1.450				
E =	0.392			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.358	1.358	1.56	1.60	**P+L, sd(W):**	**0.069**

UNIX	**SMART**			**PA**		
0.42		logKw	2.630		P, count:	3
0.70		R (**E**)=	**0.392**	0.37		
0.00		Pi (**S**)=	0.680	0.78	**P, sd:**	**0.012**
0.45		Alpha (**A**) =	**0.000**	0.00		
3.32		Beta (**B**)=	0.510	0.41	L, count:	9
		LogL16 (**L**) =	3.488	3.427		
		Vx (**V**)=	0.9267		**L, sd:**	**0.080**

LogPcalc	LogPobs
1.621	1.615

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)	1.361	1.361	1.358	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	0.874	0.874	0.858	0.000	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.629	2.629	2.630	0.000	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	logL(calc)	logL(calc)	logL(obs)	(Po-Pc)^2	
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	4.006	4.006	3.988	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.488	3.488	3.488	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.629	2.629	2.630	0.000	
Atmos Chem Phys	DB-5	0.565	-0.099	1.062	0.960	0.000	2.024	0.000	RI/100	DB-5	8.307	na		na	7.604
JAFC (1976) 24(2)	OV-1	0.422	0.000	0.672	1.155	0.000	2.067	0.000	RI/100	OV-1	8.088	8.088	8.110	0.000	
JAFC (1976) 24(6)	OV-1	0.605	-0.378	1.109	1.025	0.000	2.005	0.000	RI/100	OV-1	8.204	8.204	8.110	0.009	
JAFC (1990) 38(5)	DB-1	0.228	-0.447	1.253	1.533	-0.451	2.088	0.000	RI/100	DB-1	7.957	7.957	8.080	0.015	
JAFC (1990) 38(5)	DB-Wax	-0.548	0.707	6.479	10.014	-0.658	2.192	0.000	RI/100	DB-Wax	11.444	11.444	11.550	0.011	
JAFC (1989) 37(2)	DB-Wax	-0.435	1.072	6.781	9.721	0.000	2.013	0.000	RI/100	DB-Wax	11.617	11.617	11.510	0.011	
JAFC (1989) 37(2)	DB-1	0.447	-0.580	1.417	0.968	0.000	1.985	0.000	RI/100	DB-1	8.106	8.106	8.040	0.004	