SMILES	O=C/C=C/C
Compund No.	5402
Compund Name	**(E)-2-butenal**
Molecular Formula	C4H6O
Molecular weight	70.0898
CAS No	123-73-9
S-A/n20 =	1.437
E =	**0.387**

				P + L, count:	7
				P+L, sd:	**0.031**
				Weight:	1.00
	MD	**PA**	**ACD**		
ClogP	0.520	0.85	0.51	**P+L, sd(W):**	**0.031**

UNIX	**SMART**					
		logKw	2.633	**PA**	P, count:	2
0.387		R (**E**)=	**0.387**	**0.32**		
0.80		Pi (**S**)=	0.75	**0.72**	**P, sd:**	**0.044**
0.00		Alpha (**A**) =	**0.00**	**0.00**		
0.50		Beta (**B**)=	0.43	**0.40**	L, count:	5
2.570		LogL16 (**L**) =	2.532	**2.556**		
		Vx (**V**)=	**0.6449**		**L, sd:**	**0.031**

LogPcalc	LogPobs
1.575	1.576

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)	0.487	0.487	0.520	0.001	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.662	2.662	2.633	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	3.121	3.121	3.153	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.635	2.635	2.633	0.000	
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	6.254	6.254	6.220	0.001	
JAFC (1989) 37(3)	SE-54	0.711	-0.377	1.042	1.019	0.219	1.985	0.000	RI/100	SE-54	6.467	6.467	6.450	0.000	
JAFC (1989) 39(7)	DB-5	0.674	0.000	1.555	0.957	0.000	1.991	0.000	RI/100	DB-5	6.882	na		na	
J Sci Food Chem (:	CP-SIL-8-CB	0.490	0.000	0.962	0.863	0.259	2.030	0.000	RI/100	CP-SIL-8-CB	6.463	6.463	6.500	0.001	