SMILES	C(=C\CCO)\CC			C_w=	
Compound No.	8273			C_g=	
Compound Name	**(Z)-Hex-3-en-1ol**			**log Kw=**	
Molecular Formula	C6H12O			P + L, count:	19
Molecular weight	100.1600	**WS (mg/L)=**			
CAS No	928-96-1	**'P (mm Hg)=**		**P+L, sd:**	**0.060**
S-A/n20 =	1.440				
E =	0.335			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.400	1.397	1.67	1.61	**P+L, sd(W):**	**0.060**

UNIX	**SMART**			**PA**		
		logKw	3.654		P, count:	3
0.44	0.335	R (**E**)=	**0.335**	**0.36**		
0.55	0.48	Pi (**S**)=	0.560	**0.56**	**P, sd:**	**0.021**
0.35	0.37	Alpha (**A**) =	0.290	**0.31**		
0.42	0.59	Beta (**B**)=	0.570	**0.38**	L, count:	16
3.55	3.458	LogL16 (**L**) =	3.527	**3.563**		
		Vx (**V**)=	0.9697		**L, sd:**	**0.065**

LogPcalc	LogPobs
1.653	1.641

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)	1.422	1.422	1.397	0.001
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.112	-0.112	-0.127	0.000
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.649	3.649	3.654	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	5.061	5.061	5.051	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.665	3.665	3.654	0.000	
Flav Frag J (1999)	14 279-282	0.389	0.000	0.979	1.466	-0.309	2.061	0.000	RI/100		8.455	8.455	8.500	0.002	
JAFC (2004) 52(6)	DB-5	0.844	-0.374	1.376	0.723	0.000	1.956	0.000	RI/100	DB-5	8.598	8.598	8.520	0.006	
JAFC (2002) 50(21	CPSil-5CB	0.194	-0.505	0.955	0.886	0.000	2.119	0.000	RI/100	CPSil-5CB	8.290	8.290	8.280	0.000	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	13.789	13.789	13.680	0.012	
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	8.393	8.393	8.420	0.001	
JAFC (2004) 52(13	DB-Wax	-0.227	0.607	6.405	10.711	-0.713	2.167	0.000	RI/100	DB-Wax	13.906	13.906	13.850	0.003	
JAFC (2001) 49(3)	1345-1352	0.782	-0.451	1.312	0.808	0.000	1.975	0.000	RI/100		8.566	8.566	8.510	0.003	
Flav Frag J (1999)	HP-1	0.309	-0.579	1.155	1.227	0.000	2.059	0.000	RI/100	HP-1	8.380	8.380	8.420	0.002	
Flav Frag J (1999)	14 303-311	0.235	-0.456	1.246	1.000	0.000	2.097	0.000	RI/100		8.466	8.466	8.550	0.007	
JAFC (1994) 42(3)	DB-1	0.497	0.000	0.738	0.967	0.000	2.018	0.000	RI/100	DB-1	8.308	8.308	8.340	0.001	
Phytochemistry (1999)	52 1035-1040	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100		8.555	8.555	8.560	0.000	
Food Chemistry (2(	HP-1	0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100	HP-1	8.276	8.276	8.350	0.005	
JAFC (2001) 49(12	AT-Wax	-0.603	0.721	6.999	10.571	-1.285	2.169	0.000	RI/100	AT-Wax	13.541	13.541	13.640	0.010	
JAFC (2001) 49(12	CPSil-5CB	0.367	-0.590	1.188	1.143	-0.319	2.084	0.000	RI/100	CPSil-5CB	8.334	8.334	8.230	0.011	
"Quant Anal Frav F	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	8.617	na		na	8.470
"Quant Anal Frav F	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	13.326	na		na	13.510