SMILES	C3(C)C12C(C1/C(=C\C2)C)C(CC3)C(C)C			C_w=	
Compound No.				C_g=	
Compound Name	**Alpha-cubebene**			**log Kw=**	
Molecular Formula	C15H24			P + L, count:	15
Molecular weight	204.3500	**WS (mg/L)=**			
CAS No	17699-14-8	**/P (mm Hg)=**		**P+L, sd:**	**0.078**
S-A/n20 =	1.481				
E =	0.551			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	5.980		5.59	6.15	**P+L, sd(W):**	**0.078**

UNIX	**SMART**			**PA**		
0.81		logKw	-0.063		P, count:	3
		R (**E**)=	**0.551**	0.78		
0.39		Pi (**S**)=	0.150	0.39	**P, sd:**	**0.096**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.21		Beta (**B**)=	0.380	0.25	L, count:	12
6.68		LogL16 (**L**) =	6.379	6.994		
		Vx (**V**)=	1.8533		**L, sd:**	**0.078**

											LogPcalc	LogPobs	
											4.169	4.120	
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)	5.993	5.993	5.980	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	6.577	6.577	6.442	0.018
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.065	-0.065	-0.063	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	5.926	5.926	5.917	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	6.379	6.379	6.379	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	0.064	0.064	-0.063	0.016	
Phytochemistry (19	DB-5	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100	DB-5	13.500	13.500	13.510	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		13.565	13.565	13.660	0.009	
JAFC (2002) 50(23	HP-5MS	1.056	-0.389	1.715	0.569	0.000	1.855	0.000	RI/100	HP-5MS	12.932	na		na	13.220
JAFC (2002) 50(21	CP-SIL-5CB	0.194	-0.505	0.955	0.886	0.000	2.119	0.000	RI/100	CP-SIL-5CB	13.576	13.576	13.490	0.007	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	14.442	14.442	14.470	0.001	
RBT (2002) 50(3/4) 963		1.036	0.000	1.317	0.759	0.000	1.892	0.000	RI/100		13.303	na		na	13.510
Fanciullino et al.	DB-Wax	-0.349	1.306	6.042	9.083	0.000	2.093	0.000	RI/100	DB-Wax	14.628	14.628	14.490	0.019	
Fanciullino et al.	DB-1	0.364	0.000	0.984	1.314	0.000	2.022	0.000	RI/100	DB-1	13.410	13.410	13.320	0.008	
JAFC (2004) 52(13	DB-Wax	-0.227	0.607	6.405	10.711	-0.713	2.167	0.000	RI/100	DB-Wax	14.620	14.620	14.690	0.005	
Flav Frag J (2004)	DB-5MS	0.663	0.000	1.205	1.003	0.000	1.983	0.000	RI/100	DB-5MS	13.493	13.493	13.510	0.000	
Flav Frag J (2004)	DB-Wax	-0.199	0.893	5.848	9.166	0.000	2.107	0.000	RI/100	DB-Wax	14.611	14.611	14.630	0.000	