SMILES	[C@H]3(C)C12C(C1C(CC2)=C)[C@@H](CC3)C(C)(	C_w=	
Compound No.	70325	C_g=	
Compound Name	**ß-Cubebene**	**log Kw=**	
Molecular Formula	C15H24	P + L, count:	16
Molecular weight	204.3500	**WS (mg/L)=**	
CAS No	13744-15-5	**/P (mm Hg)=**	**P+L, sd:** **0.095**
ACD/n20 =	1.505		
E =	0.774	Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	5.980		5.48	6.14	**P+L, sd(W):**	**0.095**

UNIX	SMART					
		logKw	0.146	PA	P, count:	3
0.81		R (**E**)=	**0.551**	0.75		
0.33		Pi (**S**)=	0.160	0.35	**P, sd:**	**0.083**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.21		Beta (**B**)=	0.400	0.24	L, count:	13
6.63		LogL16 (**L**) =	6.649	6.942		
		Vx (**V**)=	1.8533		**L, sd:**	**0.101**

											LogPcalc	LogPobs	
											4.145	4.210	
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)	5.914	5.914	5.980	0.004
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	6.464	6.464	6.502	0.001
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	0.058	0.058	0.146	0.008

											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	6.193	6.193	6.126	0.004	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	6.649	6.649	6.649	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	0.130	0.130	0.146	0.000	
Phytochemistry (19	DB-5	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100	DB-5	14.052	14.052	13.890	0.026	
Flav Frag J (1999) 14	279-282	0.389	0.000	0.979	1.466	-0.309	2.061	0.000	RI/100		14.125	14.125	14.150	0.001	
JAFC (2002) 50(23	HP-5MS	1.056	-0.389	1.715	0.569	0.000	1.855	0.000	RI/100	HP-5MS	13.450	13.450	13.610	0.026	
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	14.157	14.157	14.260	0.011	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	15.088	15.088	15.240	0.023	
RBT (2002) 50(3/4)	963	1.036	0.000	1.317	0.759	0.000	1.892	0.000	RI/100		13.826	13.826	13.880	0.003	
Fanciullino et al.	DB-Wax	-0.349	1.306	6.042	9.083	0.000	2.093	0.000	RI/100	DB-Wax	15.253	15.253	15.220	0.001	
Fanciullino et al.	DB-1	0.364	0.000	0.984	1.314	0.000	2.022	0.000	RI/100	DB-1	13.965	na		na	13.740
JAFC (2004) 52(13	DB-Wax	-0.227	0.607	6.405	10.711	-0.713	2.167	0.000	RI/100	DB-Wax	15.255	na		na	17.090
Flav Frag J (2004)	DB-5MS	0.663	0.000	1.205	1.003	0.000	1.983	0.000	RI/100	DB-5MS	14.040	na		na	13.710
Flav Frag J (2004)	DB-Wax	-0.199	0.893	5.848	9.166	0.000	2.107	0.000	RI/100	DB-Wax	15.238	15.238	15.090	0.022	
Flav Frag J (2000)	HP-5MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP-5MS	13.923	13.923	13.850	0.005	
JAFC (2004) 52(6)	DB-5	0.844	-0.374	1.376	0.723	0.000	1.956	0.000	RI/100	DB-5	13.863	13.863	13.840	0.001	