SMILES	C1CC2(C3C(C1C(C)C)C2/C(=C\C3)C)C		C_w=
Compound No.	70309		C_g=
Compound Name	**(−)-α-Copaene**		**log Kw=**
Molecular Formula	C15H24		P + L, count: 17
Molecular weight	204.350	**WS (mg/L)=**	
CAS No	3856-25-5	**'P (mm Hg)=**	**P+L, sd: 0.076**
S-A/n20 =	1.490		
E =	**0.635**		Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)	
	5.980		5.00	6.17	**P+L, sd(W): 0.076**

UNIX	SMART			PA		
		logKw	0.129		P, count:	3
0.81	0.630	R (**E**)=	**0.635**	0.78		
0.39	0.13	Pi (**S**)=	0.110	0.39	**P, sd:**	**0.049**
0.00	0.00	Alpha (**A**) =	**0.000**	0.00		
0.21		Beta (**B**)=	0.420	0.25	L, count:	14
6.68	6.500	LogL16 (**L**) =	6.606	6.994		
		Vx (**V**)=	1.8533		**L, sd:**	**0.082**

LogPcalc	LogPobs
4.174	4.195

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)	5.944	5.944	5.980	0.001
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	6.503	6.503	6.477	0.001
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	0.075	0.075	0.129	0.003

											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	6.149	6.149	6.109	0.002	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	6.606	6.606	6.606	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	0.168	0.168	0.129	0.002	
Phytochemistry (19	DB-5	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100	DB-5	13.886	13.886	13.760	0.016	
Food Res Int (2001	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	13.630	13.630	13.790	0.026	
Flav Frag J (2000)	HP5-MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP5-MS	13.744	13.744	13.710	0.001	
Flav Frag J (1999)	HP-1	0.309	-0.579	1.155	1.227	0.000	2.059	0.000	RI/100	HP-1	13.670	13.670	13.650	0.000	
JAFC (1999) 47(12	CPWax-52-CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CPWax-52-CB	15.036	na		na	14.790
JAFC (1999) 47(12	CPSil-8-CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CPSil-8-CB	13.851	13.851	13.820	0.001	
RBT (2002) 50(3/4) 963		1.036	0.000	1.317	0.759	0.000	1.892	0.000	RI/100		13.679	13.679	13.770	0.008	
Flav Frag J (1999) 14 279-282		0.389	0.000	0.979	1.466	-0.309	2.061	0.000	RI/100		13.982	13.982	13.920	0.004	
JAFC (2004) 52(6)	DB-5	0.844	-0.374	1.376	0.723	0.000	1.956	0.000	RI/100	DB-5	13.679	13.679	13.710	0.001	
JAFC (2002) 50(23	HP5-MS	1.056	-0.389	1.715	0.569	0.000	1.855	0.000	RI/100	HP5-MS	13.252	na		na	13.470
JAFC (2002) 50(21	CPSil-8-CB	0.194	-0.505	0.955	0.886	0.000	2.119	0.000	RI/100	CPSil-8-CB	13.976	na		na	13.740
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	14.755	14.755	14.760	0.000	
Fanciullino et al.	DB-Wax	-0.349	1.306	6.042	9.083	0.000	2.093	0.000	RI/100	DB-Wax	14.971	14.971	14.810	0.026	
Fanciullino et al.	DB-1	0.364	0.000	0.984	1.314	0.000	2.022	0.000	RI/100	DB-1	13.830	na		na	13.490
JAFC (2004) 52(13	DB-Wax	-0.227	0.607	6.405	10.711	-0.713	2.167	0.000	RI/100	DB-Wax	14.879	14.879	14.920	0.002	