SMILES	CC(=C)[C@@H]1[C@@](C=C)(C)CC[C@@H](C1)C			C_w=	
Compound No.	70304			C_g=	
Compound Name	**ß-Elemene**			**log Kw=**	
Molecular Formula	C15H24			P + L, count:	17
Molecular weight	204.3500	**WS (mg/L)=**			
CAS No	515-13-9	**/P (mm Hg)=**		**P+L, sd:**	**0.137**
ACD/n20 =	1.501				
E =	0.752			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	6.360		5.53	6.63	**P+L, sd(W):**	**0.137**

UNIX	**SMART**			**PA**		
		logKw	-0.015		P, count:	2
0.70	0.714	R (**E**)=	**0.714**	**0.53**		
0.20	0.26	Pi (**S**)=	0.250	**0.28**	**P, sd:**	**0.258**
0.00	0.00	Alpha (**A**) =	**0.000**	**0.00**		
0.23		Beta (**B**)=	0.340	**0.32**	L, count:	15
6.37	6.552	LogL16 (**L**) =	6.564	**6.455**		
		Vx (**V**)=	1.9845		**L, sd:**	**0.129**

LogPcalc	LogPobs
3.297	3.173

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)	6.618	6.618	6.360	0.067	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.023	-0.023	-0.015	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	6.098	6.098	6.345	0.061	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	0.240	0.240	-0.015	0.065	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	6.564	6.564	6.550	0.000	
JAFC (2004) 52(6)	DB-5	0.844	-0.374	1.376	0.723	0.000	1.956	0.000	RI/100	DB-5	13.760	13.760	13.860	0.010	
Flav Frag J (1999)	14 279-282	0.389	0.000	0.989	1.435	-0.309	2.061	0.000	RI/100		14.059	14.059	13.950	0.012	
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	13.981	13.981	13.880	0.010	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	15.654	15.654	15.730	0.006	
JAFC (2002) 50(23	HP-5MS	1.056	-0.389	1.715	0.569	0.000	1.855	0.000	RI/100	HP-5MS	13.383	na		na	13.300
RBT (2002) 50(3/4)	963	1.036	0.000	1.317	0.759	0.000	1.892	0.000	RI/100		13.784	13.784	13.910	0.016	
Fanciullino et al.	DB-Wax	-0.349	1.306	6.042	9.083	0.000	2.093	0.000	RI/100	DB-Wax	15.832	15.832	15.730	0.010	
Fanciullino et al.	DB-1	0.364	0.000	0.984	1.314	0.000	2.022	0.000	RI/100	DB-1	13.882	13.882	13.700	0.033	
JAFC (2004) 52(13	DB-Wax	-0.227	0.607	6.405	10.711	-0.713	2.167	0.000	RI/100	DB-Wax	15.789	15.789	15.860	0.005	
JCA (2002) 976 26	FSOT RSL-200	0.708	0.000	0.803	1.621	0.000	1.978	0.000	RI/100	FSOT RSL-200	13.892	13.892	13.910	0.000	
Phytochemistry (19	DB-5	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100	DB-5	13.934	13.934	13.910	0.001	
Flav Frag J (2000)	HP-5MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP-5MS	13.829	13.829	13.870	0.002	
Botanica Complute	DB-1	0.555	0.000	0.906	1.847	0.000	1.997	0.000	RI/100	DB-1	13.889	13.889	13.860	0.001	