SMILES	C=1(CCC\2C(C=1)C(C/C=C/2C)C(C)C)C		C_w=
Compound No.			C_g=
Compound Name	**a-Muurolene**		**log Kw=**
Molecular Formula	C15H24		P + L, count: 19
Molecular weight	204.3500	**WS (mg/L)=**	
CAS No	31983-22-9	**VP (mm Hg)=**	**P+L, sd: 0.087**
ACD/n20 =	1.483		
E =	0.572		Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)	
	6.303		5.79	6.56	**P+L, sd(W): 0.087**

UNIX	SMART			PA		
		logKw	0.170		P, count:	3
0.79		R (**E**)=	**0.710**	0.71		
0.43		Pi (**S**)=	0.310	0.42	**P, sd:**	**0.079**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.17		Beta (**B**)=	0.330	0.29	L, count:	16
6.88		LogL16 (**L**) =	7.028	7.011		
		Vx (**V**)=	1.9189		**L, sd:**	**0.090**

LogPcalc	LogPobs
4.477	4.444

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)	6.337	6.337	6.303	0.001	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	6.959	6.959	6.858	0.010	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	0.136	0.136	0.170	0.001	

											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	6.525	6.525	6.473	0.003	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	7.028	7.028	7.028	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	0.255	0.255	0.170	0.007	
Flav Frag J (1999) 14 279-282		0.389	0.000	0.979	1.466	-0.309	2.061	0.000	RI/100		15.076	15.076	15.050	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	14.349	na		na	14.690
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	15.024	15.024	14.910	0.013	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	17.039	17.039	17.040	0.000	
JAFC (2001) 49(12	AT-Wax	-0.603	0.721	6.999	10.571	-1.285	2.169	0.000	RI/100	AT-Wax	16.899	16.899	17.040	0.020	
JAFC (2001) 49(12	CP-Sil-5CB	0.367	-0.590	1.188	1.143	-0.319	2.084	0.000	RI/100	CP-Sil-5CB	14.858	14.858	14.910	0.003	
Qual Anal Flav Fra	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	15.250	na		na	15.000
Qual Anal Flav Fra	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	17.435	17.435	17.300	0.018	
JAFC (2002) 50(18	CP-Sil-5CB	0.398	-0.470	1.055	1.252	-0.325	2.076	0.000	RI/100	CP-Sil-5CB	14.875	14.875	14.870	0.000	
JAFC (2002) 50(18	AT-Wax	-0.400	0.547	6.558	10.358	-0.939	2.171	0.000	RI/100	AT-Wax	16.970	na		na	14.570
Phytochemistry (19	DB-5	0.711	-0.293	1.114	0.864	0.000	2.004	0.000	RI/100	DB-5	14.933	14.933	14.980	0.002	
Zeit. Natur. (2002)	HP-5MS	0.600	0.000	0.965	1.699	0.000	1.998	0.000	RI/100	HP-5MS	14.942	14.942	14.790	0.023	
Flav Frag J (2000)	HP-5MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP-5MS	14.837	14.837	14.980	0.021	
Flav Frag J (1999)	HP-1	0.309	-0.579	1.155	1.227	0.000	2.059	0.000	RI/100	HP-1	14.727	14.727	14.780	0.003	
Flav Frag J (2004)	DB-5MS	0.663	0.000	1.205	1.003	0.000	1.983	0.000	RI/100	DB-5MS	14.974	14.974	15.020	0.002	
Flav Frag J (2004)	DB-Wax	-0.199	0.893	5.848	9.166	0.000	2.107	0.000	RI/100	DB-Wax	17.057	17.057	16.970	0.007	