SMILES	C(=C/CC\C(=C\CCC(C)=O)C)(\C)C	C_w=	
Compound No.		C_g=	
Compound Name	**Geranyl acetone**	**log Kw=**	
Molecular Formula	C13H22O	P + L, count:	21
Molecular weight	194.3100	**WS (mg/L)=**	
CAS No	689-67-8	**VP (mm Hg)=**	**P+L, sd:** **0.096**
Beil/n20 =	1.468		
E =	**0.428**	Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	3.854		4.06	4.13	**P+L, sd(W):**	**0.096**

UNIX	SMART			PA		
		logKw	3.295		P, count:	2
0.57		R (**E**)=	**0.428**	0.47		
0.76		Pi (**S**)=	0.750	0.80	**P, sd:**	**0.155**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.46		Beta (**B**)=	0.770	0.53	L, count:	19
6.70		LogL16 (**L**) =	6.499	6.610		
		Vx (**V**)=	1.8700		**L, sd:**	**0.094**

	LogPcalc	LogPobs
	3.637	3.574

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)	4.006	4.006	3.854	0.023	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.267	3.267	3.295	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	7.011	7.011	7.149	0.019	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.461	3.461	3.295	0.027	
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	14.736	14.736	14.580	0.024	
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	14.597	14.597	14.600	0.000	
JAFC (2000) 48(6)	DB-5	0.307	-0.424	1.298	1.348	0.000	2.088	0.000	RI/100	DB-5	14.669	14.669	14.600	0.005	
Food Res Int (2001	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	14.527	14.527	14.580	0.003	
JAFC (1981) 29(2)	OV-101	0.447	0.000	0.776	0.829	0.306	2.022	0.000	RI/100	OV-101	14.406	14.406	14.310	0.009	
JAFC (1981) 29(2)	CW-20M	-0.769	0.537	6.515	9.776	-0.581	2.193	0.000	RI/100	CW-20M	18.152	18.152	18.110	0.002	
JAFC (1983) 31(6)	DB-1	0.624	0.000	0.548	0.545	0.404	1.991	0.000	RI/100	DB-1	14.286	14.286	14.270	0.000	
JAFC (1990) 38(2)	DB-1	0.558	-0.541	0.902	0.922	0.000	2.047	0.000	RI/100	DB-1	14.306	14.306	14.280	0.001	
JAFC (1990) 38(1)	DB-1	-0.171	-0.960	1.669	1.754	-0.444	2.164	0.000	RI/100	DB-1	14.392	14.392	14.280	0.013	
JAFC (1993) 41(11	Ultra-2	0.304	-0.386	1.527	1.585	0.000	2.038	0.000	RI/100	Ultra-2	14.529	14.529	14.620	0.008	
JAFC (1995) 43(7)	DB-1	0.313	0.000	0.637	0.865	0.241	2.058	0.000	RI/100	DB-1	14.351	14.351	14.290	0.004	
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	14.089	na		na	14.290
JAFC (2002) 50(5)	BPX-5	0.411	0.000	1.247	1.297	0.169	2.033	0.000	RI/100	BPX-5	14.689	14.689	14.640	0.002	
JAFC (2005) 53(8)	HP-1	0.545	0.000	0.869	1.424	0.000	2.005	0.000	RI/100	HP-1	14.227	14.227	14.280	0.003	
JAFC (2005) 53(8)	Innowax	0.198	0.950	5.836	9.664	0.000	2.043	0.000	RI/100	Innowax	18.259	na		na	18.500
JAFC (2001) 49(3)	1345-1352	0.782	-0.451	1.312	0.808	0.000	1.975	0.000	RI/100		14.409	14.409	14.480	0.005	
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	14.156	14.156	14.290	0.018	
JAFC (2001) 49(12	AT-Wax	-0.549	0.959	6.556	10.322	-0.839	2.171	0.000	RI/100	AT-Wax	18.242	18.242	18.280	0.001	
JAFC (2001) 49(12	CP-Sil-5CB	0.491	-0.511	1.164	1.206	-0.377	2.056	0.000	RI/100	CP-Sil-5CB	14.217	14.217	14.340	0.015	