SMILES	C(C(CCC\C(=C\CO)C)C)CCC(CCCC(C)C)C			C_w=	0.000
Compound No.	8299			C_g=	0.000
Compound Name	**Phytol**			**log Kw=**	#DIV/0!
Molecular Formula	C20H40O			P + L, count:	6
Molecular weight	296.5310	**WS=**			
CAS No	150-86-7	**VP=**		**P+L, sd:**	**0.123**
S-A/n20 =	1.463				
E =	**0.297**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	8.480	8.483	7.52	8.66	**P+L, sd(W):**	**0.123**

UNIX	**SMART**			**PA**		
0.41	0.297	logKw	1.231		P, count:	0
0.42	0.41	R (**E**)=	**0.297**	**0.27**		
0.35	0.38	Pi (**S**)=	0.390	**0.38**	**P, sd:**	**0.000**
0.47	0.48	Alpha (**A**) =	0.270	**0.31**		
9.82		Beta (**B**)=	0.370	**0.45**	L, count:	6
		LogL16 (**L**) =	9.632	**9.685**		
		Vx (**V**)=	**2.9423**		**L, sd:**	**0.123**

											LogPcalc	LogPobs		
											#DIV/0!	#DIV/0!		
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)	9.795	na		na	MD
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	0.435	na		na	
											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	9.822	na		na	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	0.827	na		na	
JAFC (1985) 33(3)	SE-54	0.591	-1.481	-4.045	1.859	7.894	2.002	0.000	RI/100	SE-54	21.280	21.280	21.300	0.000	
JAFC (1992) 40(4)	SupelcoWax TM-10	0.127	0.000	6.664	9.249	0.000	2.034	0.000	RI/100	SupelcoWax TM-10	24.815	na		na	26.110
JAFC (1992) 40(4)	HP-1	0.557	-0.770	1.501	1.252	0.000	2.003	0.000	RI/100	HP-1	20.545	na		na	21.250
JAFC (2001) 49(12	AT-Wax	-0.603	0.721	6.999	10.571	-1.285	2.169	0.000	RI/100	AT-Wax	25.611	25.611	25.710	0.010	
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	20.919	na		na	20.660
JAFC (2001) 49(12	AT-Wax	-0.549	0.959	6.556	10.322	-0.839	2.171	0.000	RI/100	AT-Wax	25.680	25.680	25.570	0.012	
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	20.783	na		na	21.010
Flav Frag J (2000)	HP-5 MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP-5 MS	20.641	na		na	21.220
Flav Frag J (1999)	HP-1	0.309	-0.579	1.155	1.227	0.000	2.059	0.000	RI/100	HP-1	20.751	20.751	20.910	0.025	
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	20.884	20.884	21.010	0.016	
JAFC (2002) 50(18	AT-Wax	-0.400	0.547	6.558	10.358	-0.939	2.171	0.000	RI/100	AT-Wax	25.680	25.680	25.570	0.012	