SMILES	c1(cc(ccc1O)CC=C)OC
Compund No.	16841
Compund Name	**Eugenol**
Molecular Formula	C10H12O2
Molecular weight	164.2011
CAS No	97-53-0
S-A/n20 =	1.541
E =	**0.946**

	MD	PA	ACD
ClogP	2.397	2.58	2.40

P + L, count:	16
P+L, sd:	**0.066**
Weight:	1.00
P+L, sd(W):	**0.066**
P, count:	2
P, sd:	**0.067**
L, count:	14
L, sd:	**0.068**

UNIX	**SMART**			PA
		logKw	5.307	
1.02	0.946	R (**E**)=	**0.946**	0.98
0.78	0.99	Pi (**S**)=	0.95	0.96
0.29	0.22	Alpha (**A**) =	0.28	0.28
0.62	0.51	Beta (**B**)=	0.71	0.53
5.88	6.061	LogL16 (**L**) =	5.872	6.046
		Vx (**V**)=	**1.3544**	

LogPcalc	LogPobs
3.819	3.788

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)	2.337	2.337	**2.270**	0.004
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.302	5.302	5.307	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	7.516	7.516	7.577	0.004
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	5.373	5.373	5.307	0.004
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	20.991	na		na
JAFC (1992) 40(4)	HP-1	0.557	-0.770	1.501	1.252	0.000	2.003	0.000	RI/100	HP-1	13.367	13.367	13.440	0.005
FC (1999) 47(12) 51	CPWax-52-CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CPWax-52-CB	21.532	21.532	21.550	0.000
; (2000) 48(6) 2395-	DB-5	0.307	-0.424	1.298	1.348	0.000	2.088	0.000	RI/100	DB-5	13.777	na		na
; (2001) 49(6) 2924-	DB-Wax	-2.488	0.000	8.261	11.077	2.463	2.106	0.000	RI/100	DB-Wax	22.577	na		na
em (1993) 65(21) 31	OV-101	0.426	-0.311	1.145	1.189	0.000	2.034	0.000	RI/100	OV-101	13.496	13.496	13.510	0.000
em (1993) 65(21) 31	CW-20M	0.249	1.200	6.184	8.439	-0.765	2.027	0.000	RI/100	CW-20M	20.981	20.981	21.030	0.002
Chem (2003) 80 35	HP-1	0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100	HP-1	13.226	13.226	13.190	0.001
Food Research Int	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	13.694	13.694	13.640	0.003
emistry (1999) 52 1(	DB-5	0.965	-0.353	1.129	0.826	0.000	1.957	0.000	RI/100	DB-5	13.426	13.426	13.560	0.018
FC (1999) 47(12) 51	CPSIL-8CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CPSIL-8CB	13.621	13.621	13.570	0.003
tative Analysis Flav.	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	13.889	na		na
tative Analysis Flav.	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	21.106	21.106	21.030	0.006
; (2004) 52(6) 1601-	DB-5	0.844	-0.374	1.376	0.723	0.000	1.956	0.000	RI/100	DB-5	13.485	13.485	13.540	0.003
Frag J. (2003) 18 46	DB-5	0.850	0.000	0.951	1.143	0.000	1.970	0.000	RI/100	DB-5	13.641	13.641	13.560	0.007
(2001) 49(10) 4818	DB-Wax	-1.301	0.000	7.705	11.075	0.000	2.181	0.000	RI/100	DB-Wax	21.926	21.926	21.860	0.004