SMILES	c1(ccc(c(c1)OC)O)C=O				
Compund No.	16834				
Compund Name	**Vanillin**				
Molecular Formula	$C_8H_8O_3$			P + L, count:	33
Molecular weight	152.147				
CAS No	121-33-5			**P+L, sd:**	**0.065**
ACD/n20 =	1.587				
E =	1.124			Weight:	1.00
	MD	**PA**	**ACD**		
ClogP	1.275	1.170	1.19	**P+L, sd(W):**	**0.065**

UNIX	**SMART**					
		logKw	6.422	PA	P, count:	16
1.020	1.040	R (**E**)=	1.028	0.960		
1.40	1.33	Pi (**S**)=	1.28	1.46	**P, sd:**	**0.050**
0.50	0.29	Alpha (**A**) =	0.33	0.34		
0.78	0.69	Beta (**B**)=	0.68	0.69	L, count:	17
5.630	5.709	LogL16 (**L**) =	5.731	5.924		
		Vx (**V**)=	1.1313		**L, sd:**	**0.079**

											LogPcalc	LogPobs		
												0.810	0.816	
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)	1.308	1.308	**1.310**	0.000
b	Hexanol	0.143	0.718	-0.980	0.145	-3.214	0.000	3.403	P	Hexanol	1.355	1.355	1.450	0.009
b	Decanol	0.008	0.485	-0.974	0.015	-3.798	0.000	3.945	P	Decanol	1.164	1.164	1.190	0.001
Jamie	Trichloromethane	0.327	0.157	-0.391	-3.191	-3.437	0.000	4.191	P	Trichloromethane	1.356	1.356	1.420	0.004
CTET-1	Tetrachloromethane	0.260	0.573	-1.254	-3.558	-4.588	0.000	4.589	P	CCl4 Sept 98	0.166	0.166	0.200	0.001
Caroline	Hexane August 98	0.361	0.579	-1.723	-3.599	-4.764	0.000	4.344	P	Hexane August 98	-0.736	-0.736	-0.700	0.001
Caroline	Heptane August 98	0.325	0.670	-2.061	-3.317	-4.733	0.000	4.543	P	Heptane August 98	-0.771	-0.771	-0.720	0.003
Caroline	Octane August 98	0.223	0.642	-1.647	-3.480	-5.067	0.000	4.526	P	Octane August 98	-0.671	-0.671	-0.700	0.001
Caroline	Decane August 98	0.160	0.585	-1.734	-3.435	-5.078	0.000	4.582	P	Decane August 98	-0.833	-0.833	-0.800	0.001
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	6.400	6.400	6.422	0.001
CYC-1	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577	P	Cyclohexane/Dec 98	-0.564	-0.564	-0.660	0.009
BENZ-1	Benzene	0.142	0.464	-0.588	-3.099	-4.625	0.000	4.491	P	Benzene/Dec/1997 (25celi	0.802	0.802	0.800	0.000
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	0.655	0.655	0.640	0.000
AMAL	Bromobenzene	-0.130	0.394	-0.280	-3.331	-4.640	0.000	4.583	P	Bromobenzene	0.869	0.869	0.810	0.004
a	Nitrobenzene	-0.181	0.576	0.003	-2.356	-4.420	0.000	4.263	P	Nitrobenzene	1.475	1.475	1.460	0.000
a	Diethyl ether	0.248	0.561	-1.016	-0.226	-4.553	0.000	4.075	P	Diethyl ether/ Wet/2002	0.987	0.987	0.930	0.003

											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	7.753	7.753	7.732	0.000
	Chloroform	0.116	-0.467	1.203	0.138	1.432	0.994	0.000	L	CHCl3/Wet/25.8.97	7.883	7.883	7.842	0.002
CTET-1	Tetrachloromethane	0.282	-0.303	0.460	0.000	0.000	1.047	0.000	L	CCl4/Sept 98	6.559	6.559	6.622	0.004
Caroline	Hexane	0.292	-0.169	0.000	0.000	0.000	0.979	0.000	L	Hexane	5.729	5.729	5.722	0.000
Caroline	Heptane	0.275	-0.162	0.000	0.000	0.000	0.983	0.000	L	Heptane	5.743	5.743	5.702	0.002
Caroline	Octane	0.215	-0.049	0.000	0.000	0.000	0.967	0.000	L	Octane	5.707	5.707	5.722	0.000
Caroline	Decane	0.156	-0.143	0.000	0.000	0.000	0.989	0.000	L	Decane	5.677	5.677	5.622	0.003
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	6.396	6.396	6.422	0.001
BENZ-1	Benzene	0.107	-0.313	1.053	0.457	0.169	1.020	0.000	L	Benzene/Dec 97	7.241	7.241	7.222	0.000
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	7.112	7.112	7.062	0.003
	Nitrobenzene	-0.273	0.039	1.803	1.231	0.000	0.929	0.000	L	Nitrobenzene	7.801	7.801	7.882	0.007
	Diethyl ether / Wet/200	0.206	-0.169	0.873	3.402	0.000	0.882	0.000	L	Diethyl ether/ Wet /2002	7.325	7.325	7.352	0.001
JAFC (2000) 48(2)	DB-Wax	-1.307	0.523	9.055	10.206	0.000	1.977	0.000	RI/100	DB-Wax	25.494	25.494	25.480	0.000
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	13.422	13.422	13.450	0.001
JAFC (1998) 46(2)	InnoWax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	InnoWax	24.208	na		na
JAFC (1990) 38(1)	HP-5	0.025	-0.220	1.288	1.203	0.000	2.127	0.000	RI/100	HP-5	14.032	14.032	14.120	0.008
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	13.714	13.714	13.490	0.050
JCA (1999) 848 21!	SE-30	0.660	-0.295	0.934	0.889	-0.539	2.070	0.000	RI/100	SE-30	13.343	13.343	13.479	0.018