SMILES	c1ccc2c(c1)\C=C/C(O2)=O
Compund No.	18622
Compund Name	**Coumarin**
Molecular Formula	C9H6O2
Molecular weight	146.1427
CAS No	91-64-5
ACD/n20 =	1.594
E =	1.122

	MD	PA	ACD
ClogP	1.412	1.66	1.39

P + L, count:	11
P+L, sd:	**0.070**
Weight:	1.00
P+L, sd(W):	**0.070**
P, count:	3
P, sd:	**0.127**
L, count:	8
L, sd:	**0.050**

UNIX	SMART			PA
		logKw	5.580	
1.37	1.060	R (**E**)=	1.231	1.13
1.30	1.76	Pi (**S**)=	1.680	1.30
0.00	0.00	Alpha (**A**) =	**0.000**	0.03
0.56	0.43	Beta (**B**)=	0.520	0.56
5.60	5.809	LogL16 (**L**) =	6.019	5.661
		Vx (**V**)=	**1.0619**	

LogPcalc	LogPobs
2.485	2.483

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)	1.260	1.260	**1.390**	0.017	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.593	5.593	5.580	0.000	
CYC-1	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577	P	Cyclohexane/Dec 98	0.602	0.602	0.480	0.015	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	logL(calc)	logL(calc)	logL(obs)	(Po-Pc)^2
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	6.903	6.903	6.970	0.005
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	5.570	5.570	5.580	0.000
CYC-1	Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013	0.000	L	Cyclohexane/Dec/98	6.125	6.125	6.060	0.004
Anal Chem (1993)	OV-101	0.426	-0.311	1.145	1.189	0.000	2.034	0.000	RI/100	OV-101	14.210	14.210	14.180	0.001
JAFC (1992) 40(4)	Supelcowax TM10	0.127	0.000	6.664	9.249	0.000	2.034	0.000	RI/100	Supelcowax TM10	23.565	23.565	23.580	0.000
JAFC (1992) 40(4)	HP-1	0.557	-0.770	1.501	1.252	0.000	2.003	0.000	RI/100	HP-1	14.187	14.187	14.140	0.002
Phytochem (1999)	DB-5	0.965	-0.353	1.129	0.826	0.000	1.957	0.000	RI/100	DB-5	14.207	14.207	14.280	0.005
"Qualitative Anal. F	CW 20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW 20M	23.614	23.614	23.610	0.000
"Qualitative Anal. F	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	14.707	na		na
Anal Chem (1993)	CW 20M	0.249	1.200	6.184	8.439	-0.765	2.027	0.000	RI/100	CW 20M	23.918	na		na