SMILES	C\C1=C\C(CC(C1)(C)C)=O
Compund No.	5791
Compund Name	**Isophorone**
Molecular Formula	C9H14O
Molecular weight	138.2069
CAS No	78-59-1
S-A/n20 =	1.476
E =	**0.511**

	MD	PA	ACD
ClogP	2.088	1.91	2.07

P + L, count:	12
P+L, sd:	**0.079**
Weight:	1.00
P+L, sd(W):	**0.079**
P, count:	2
P, sd:	**0.054**
L, count:	10
L, sd:	**0.086**

UNIX	SMART			PA
0.61	0.511	logKw	3.340	
0.75	1.13	R (**E**)=	**0.511**	0.51
0.00	0.00	Pi (**S**)=	0.88	1.12
0.48	0.50	Alpha (**A**) =	**0.00**	0.00
4.74	4.697	Beta (**B**)=	0.59	0.53
		LogL16 (**L**) =	4.828	4.740
		Vx (**V**)=	**1.2408**	

LogPcalc	LogPobs
2.730	2.714

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)	2.139	2.139	2.088	0.003	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.322	3.322	3.340	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	5.412	5.412	5.428	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.375	3.375	3.340	0.001	
JAFC (1998) 46(2)	CP-SIL5 CB	0.572	0.000	1.006	1.348	-0.654	2.024	0.000	RI/100	CP-SIL5 CB	10.843	10.843	10.990	0.022	
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	11.428	na		na	
Food Chem (1999) 64 3-11		0.045	-0.609	1.664	1.596	-0.555	2.067	0.000	RI/100		10.850	10.850	10.970	0.014	
Food Research Int	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	11.325	11.325	11.180	0.021	
Phytochem (1999)	DB-5	0.965	-0.353	1.129	0.826	0.000	1.957	0.000	RI/100	DB-5	11.226	11.226	11.190	0.001	
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	10.945	10.945	10.890	0.003	
Flav Frag J. (2003)	DB-5	0.850	0.000	0.951	1.143	0.000	1.970	0.000	RI/100	DB-5	11.198	11.198	11.200	0.000	
JAFC (2001) 49(12	AT-Wax	-0.549	0.959	6.556	10.322	-0.839	2.171	0.000	RI/100	AT-Wax	15.697	15.697	15.710	0.000	
JAFC (2001) 49(12	CP-SIL5 CB	0.491	-0.511	1.164	1.206	-0.377	2.056	0.000	RI/100	CP-SIL5 CB	10.958	10.958	10.900	0.003	