SMILES	C(=C/C(C)=O)\C=1C(C)(C)CCCC=1C
Compund No.	70682
Compund Name	**B-Ionone**
Molecular Formula	$C_{13}H_{20}O$
Molecular weight	192.2973
CAS No	79-77-6
Handbook/n20 =	1.5198
E =	0.892

P + L, count:	12
P+L, sd:	**0.107**
Weight:	1.00
P+L, sd(W):	**0.107**

P*	ClogP(MD)	ClogP(PA)	ClogP(ACD)
3.720	3.770	3.70	3.85

UNIX	SMART			PA		
		logKw	3.666		P, count:	2
0.76	0.875	R (**E**)=	**0.892**	0.88		
0.83	0.90	Pi (**S**)=	0.780	0.90	**P, sd:**	**0.136**
0.00	0.00	Alpha (**A**) =	0.000	0.00		
0.50	0.74	Beta (**B**)=	0.760	0.50	L, count:	10
6.65	7.150	LogL16 (**L**) =	6.758	6.758		
		Vx (**V**)=	**1.7614**		**L, sd:**	**0.109**

LogPcalc	LogPobs
3.756	3.693

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)	3.856	3.856	**3.720**	0.018
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.657	3.657	3.666	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	7.241	7.241	7.386	0.021
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.821	3.821	3.666	0.024
C (1998) 46(2) 611	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	14.580	14.580	14.480	0.010
C (2000) 48(2) 400	DB-Wax	-1.307	0.523	9.055	10.206	0.000	1.977	0.000	RI/100	DB-Wax	19.582	19.582	19.580	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	15.051	15.051	14.910	0.020
Res Int (2001) 34	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	14.847	14.847	14.890	0.002
Anal. Flavour and	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	19.715	na		na
Anal. Flavour and	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	15.217	na		na
C (1985) 33(2) 249	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	14.516	14.516	14.650	0.018
C (1990) 38(2) 471	DB-1	0.558	-0.541	0.902	0.922	0.000	2.047	0.000	RI/100	DB-1	14.612	14.612	14.590	0.000
/ Frag J (2000) 15	HP-5 MS	0.650	-0.301	1.381	1.458	0.000	1.988	0.000	RI/100	HP-5 MS	14.893	14.893	14.820	0.005
Flav Frag J (2003)	AT-Wax	-0.913	0.945	6.681	10.737	0.000	2.214	0.000	RI/100	AT-Wax	20.102	na		na
Flav Frag J (2003)	CP-SIL-5CB	0.347	-0.592	1.179	1.113	-0.341	2.092	0.000	RI/100	CP-SIL-5CB	14.616	14.616	14.700	0.007

i M.H.Abraham, K.Takacs-Novak and R.C.Mitchell, J.Pharm.Sci., 1997, 86,