SMILES	C(/C(C)=O)=C\C	C_w=	
Compound No.	5783	C_g=	
Compound Name	**Pent-3-en-2-one**	**log Kw=**	
Molecular Formula	C5H8O	P + L, count:	18
Molecular weight	84.1200	**WS (mg/L)=**	
CAS No	625-33-2	**'P (mm Hg)=**	**P+L, sd:** **0.073**
S-A/n20 =	1.437		
E =	0.359	Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
0.520	0.520	0.516	0.78	0.56	**P+L, sd(W):**	**0.073**

UNIX	**SMART**			**PA**		
		logKw	3.231		P, count:	4
0.42		R (**E**)=	**0.359**	0.37		
0.70		Pi (**S**)=	0.820	0.78	**P, sd:**	**0.068**
0.00		Alpha (**A**) =	**0.000**	0.00		
0.45		Beta (**B**)=	0.550	0.41	L, count:	14
2.82		LogL16 (**L**) =	2.933	2.933		
		Vx (**V**)=	0.7858		**L, sd:**	**0.077**

LogPcalc	LogPobs
0.862	0.818

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)	0.519	0.519	0.520	0.000	P*
Caroline	Heptane August 98	0.325	0.670	-2.061	-3.317	-4.733	0.000	4.543	P	Heptane August 98	-0.159	-0.159	-0.180	0.000	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.195	-0.195	-0.299	0.011	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.284	3.284	3.231	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	3.687	3.687	3.751	0.004	
Caroline	Heptane	0.275	-0.162	0.000	0.000	0.000	0.983	0.000	L	Heptane	3.100	3.100	3.051	0.002	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	2.933	2.933	2.933	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.298	3.298	3.231	0.004	
JAFC (1993) 41(11) 2056-2062		0.504	0.000	0.458	0.000	0.885	2.003	0.000	RI/100		7.241	7.241	7.100	0.020	
JAFC (1984) 32(5) 1011-1015		0.601	-0.257	0.942	1.309	0.000	1.996	0.000	RI/100		7.135	7.135	7.170	0.001	
Int Dair J (2001) 11	SPB-1	1.257	-1.221	1.255	1.627	-1.671	2.027	0.000	RI/100	SPB-1	6.873	na		na	7.160
Flav Frag J (2003)	AT-Wax	-0.913	0.945	6.681	10.737	0.000	2.214	0.000	RI/100	AT-Wax	11.398	na		na	11.110
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	7.049	7.049	6.970	0.006	
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	7.124	7.124	7.150	0.001	
JAFC (2002) 50(21	CP-SIL-5CB	0.194	-0.505	0.955	0.886	0.000	2.119	0.000	RI/100	CP-SIL-5CB	7.010	7.010	6.980	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	7.129	7.129	7.130	0.000	
JAFC (1998) 46(12	DB-5	0.679	0.000	1.070	1.587	0.000	1.994	0.000	RI/100	DB-5	7.404	7.404	7.500	0.009	
JAFC (2002) 50(7) 2010-2015		0.138	0.965	5.960	8.691	0.000	2.089	0.000	RI/100		11.498	11.498	11.420	0.006	
JAFC (2001) 49(11	HP-Wax	-0.795	1.997	6.214	9.991	0.000	2.121	0.000	RI/100	HP-Wax	11.238	11.238	11.380	0.020	
JAFC (2001) 49(3)	HP-Wax	-1.473	1.389	7.264	11.276	0.000	2.192	0.000	RI/100	HP-Wax	11.411	11.411	11.380	0.001	