SMILES	CC(C(O)C)=O			C_w=	
Compund No.	8470			C_g=	
Compound Name	**3-hydroxybutan-2-one (Acetoin)**			**log Kw=**	
Molecular Formula	C4H8O2			P + L, count:	24
Molecular weight	88.1051	**WS=**			
CAS No	513-86-0	**VP=**		**P+L, sd:**	**0.074**
S-A/n20 =	1.417				
E =	**0.289**			Weight:	1.00

P*	**ClogP**	**ClogP(MD)**	**ClogP(PA)**	**ClogP(ACD)**		
	-0.200	-0.204	-0.31	-0.43	**P+L, sd(W):**	**0.074**

UNIX	**SMART**			**PA**		
		logKw	4.872		P, count:	2
0.43	0.289	R (**E**)=	**0.289**	0.29		
0.79	0.71	Pi (**S**)=	0.690	0.71	**P, sd:**	**0.032**
0.19	0.13	Alpha (**A**) =	0.270	0.13		
0.68	0.74	Beta (**B**)=	0.740	0.74	L, count:	22
2.66	2.771	LogL16 (**L**) =	2.702	2.771		
		Vx (**V**)=	**0.7466**		**L, sd:**	**0.077**

											LogPcalc	LogPobs		
											2.357	2.334		
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)	-0.181	-0.181	-0.204	0.001	MD
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.895	4.895	4.872	0.001	
											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	4.618	4.618	4.668	0.003	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.900	4.900	4.872	0.001	
JAFC (1998) 46(12	DB-5	0.679	0.000	1.070	1.587	0.000	1.994	0.000	RI/100	DB-5	7.234	7.234	7.160	0.005	
Food Chem (1999) 64	3-11	0.045	-0.609	1.664	1.596	-0.555	2.067	0.000	RI/100		6.623	6.623	6.660	0.001	
Talanta (2003) 60 7	BPX-5	0.747	-0.452	1.223	1.642	0.000	1.977	0.000	RI/100	BPX-5	7.246	7.246	7.100	0.021	
JAFC (1981) 29(2)	OV-101	0.447	0.000	0.776	0.829	0.306	2.022	0.000	RI/100	OV-101	6.896	na		na	7.140
JAFC (1981) 29(2)	CW-20M	-0.769	0.537	6.515	9.776	-0.581	2.193	0.000	RI/100	CW-20M	12.017	na		na	12.630
JAFC (1981) 29(1)	CW-20M	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20M	12.637	12.637	12.640	0.000	
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	6.895	6.895	6.920	0.001	
JAFC (1990) 38(1)	HP-5	0.025	-0.220	1.288	1.203	0.000	2.127	0.000	RI/100	HP-5	6.922	6.922	7.060	0.019	
JAFC (1991) 39(9)	DB_1	0.637	-0.922	1.725	1.088	-0.644	2.021	0.000	RI/100	DB_1	6.839	6.839	6.800	0.002	
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	6.883	6.883	6.820	0.004	
Food Chem (2004)	CP-SIL-8CB	0.532	-0.473	1.552	1.340	-0.344	2.030	0.000	RI/100	CP-SIL-8CB	7.059	7.059	7.110	0.003	
JAFC (1995) 43(7)	DB-1	0.313	0.000	0.637	0.865	0.241	2.058	0.000	RI/100	DB-1	6.725	6.725	6.740	0.000	
JAFC (1994) 42(3)	DB-1	0.497	0.000	0.738	0.967	0.000	2.018	0.000	RI/100	DB-1	6.720	6.720	6.740	0.000	
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	7.043	na		na	6.740
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	7.179	7.179	7.170	0.000	
JAFC (1999) 47(12	CPWax-52CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CPWax-52CB	12.393	na		na	12.820
JAFC (1999) 47(12	CP-SIL-8CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CP-SIL-8CB	7.040	7.040	7.070	0.001	
JCA (2000) 905 23	CP-SIL-8CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-SIL-8CB	7.063	7.063	7.170	0.011	
JAFC (2001) 49(12	AT-Wax	-0.549	0.959	6.556	10.322	-0.839	2.171	0.000	RI/100	AT-Wax	12.284	na		na	12.720
JAFC (2001) 49(12	CP-SIL-5CB	0.491	-0.511	1.164	1.206	-0.377	2.056	0.000	RI/100	CP-SIL-5CB	6.749	6.749	6.670	0.006	
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	7.145	7.145	7.200	0.003	
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	6.672	6.672	6.670	0.000	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	12.605	12.605	12.730	0.016	
JAFC (2005) 53(8)	DB-5MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB-5MS	8.107	na		na	7.150
Flav Frag J (2003)	AT-Wax	-0.913	0.945	6.681	10.737	0.000	2.214	0.000	RI/100	AT-Wax	12.852	12.852	12.700	0.023	
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	6.690	6.690	6.620	0.005	