SMILES	C(COC(C)=O)(C)=O			C_w=	
Compound No.	6450			C_g=	
Compound Name	**Acetol acetate (2-Oxopropyl acetate)**			**log Kw=**	
Molecular Formula	C5H8O3			P + L, count:	8
Molecular weight	116.1200	**WS (mg/L)=**			
CAS No	592-20-1	**VP (mm Hg)=**		**P+L, sd:**	**0.030**
Beil/n20 =	1.415				
E =	**0.229**			Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	-0.196	-0.196	0.18	0.33	**P+L, sd(W):** **0.030**

UNIX	**SMART**			**PA**		
0.32		logKw	4.820		P, count:	2
1.04		R (**E**)=	**0.229**	**0.28**		
0.00		Pi (**S**)=	0.980	**1.07**	**P, sd:**	**0.013**
0.77		Alpha (**A**) =	**0.000**	**0.00**		
3.47		Beta (**B**)=	0.820	**0.67**	L, count:	6
		LogL16 (**L**) =	3.443	**3.554**		
		Vx (**V**)=	0.9032		**L, sd:**	**0.035**

											LogPcalc	LogPobs		
											2.306	2.312		
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)	-0.209	-0.209	-0.196	0.000	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.821	4.821	4.820	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	4.623	4.623	4.624	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.820	4.820	4.820	0.000	
JAFC (2000) 905 2	CP-Sil-5CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-Sil-5CB	8.687	8.687	8.670	0.000	
JAFC (1981) 29(1)	CW-20M	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20M	13.487	na		na	12.870
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	8.355	8.355	8.390	0.001	
JAFC (1998) 46(6)	DB-1	1.589	0.000	0.742	0.824	0.000	1.744	0.000	RI/100	DB-1	8.320	8.320	8.260	0.004	
JAFC (1999) 47(2)	DB-1	0.782	0.000	0.904	0.513	0.000	1.940	0.000	RI/100	DB-1	8.346	8.346	8.380	0.001	