SMILES	CCOC(C(O)C)=O			C_w=	
Compound No.	**8504**			C_g=	
Compound Name	**Ethyl lactate**			**log Kw=**	
Molecular Formula	C5H10O3			P + L, count:	12
Molecular weight	118.1300	**WS (mg/L)=**			
CAS No	97-64-3	**VP (mm Hg)=**		**P+L, sd:**	**0.047**
S-A/n20 =	1.413				
E =	**0.205**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	0.551	0.331	0.28	-0.19	**P+L, sd(W):**	**0.047**

Methyl-Lac	**SD 0.017**								
	4.468	**UNIX**	**SMART**	logKw	4.432	**PA**	P, count:	3
0.258	**0.205**	0.36		R (**E**)=	**0.205**	0.20		
0.740	0.600	0.68		Pi (**S**)=	0.680	0.62	**P, sd:**	**0.069**
0.100	0.250	0.10		Alpha (**A**) =	0.200	0.17		
0.790	0.760	0.68		Beta (**B**)=	0.760	0.67	L, count:	9
2.944	3.306	3.06		LogL16 (**L**) =	3.297	2.943		
0.805	0.9462			Vx (**V**)=	0.9462		**L, sd:**	**0.043**

LogPcalc	LogPobs
1.283	1.283

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)	0.472	0.472	0.551	0.006	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-1.099	-1.099	-1.134	0.001	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.477	4.477	4.432	0.002	

											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	4.904	4.904	4.983	0.006	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.297	3.297	3.297	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.500	4.500	4.432	0.005	
JAFC (2001) 49(12	AT-Wax	-0.603	0.721	6.999	10.571	-1.285	2.169	0.000	RI/100	AT-Wax	12.594	na		na	13.330
JAFC (2001) 49(12	CP-Sil-5CB	0.367	-0.590	1.188	1.143	-0.319	2.084	0.000	RI/100	CP-Sil-5CB	7.912	7.912	7.870	0.002	
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	7.904	7.904	7.870	0.001	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	13.004	na		na	13.330
Flav Frag J (2003)	AT-Wax	-0.913	0.945	6.681	10.737	0.000	2.214	0.000	RI/100	AT-Wax	13.272	13.272	13.290	0.000	
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	7.889	7.889	7.870	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	13.082	13.082	13.090	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	8.048	8.048	8.060	0.000	