SMILES C(C)CC(C)C=O

Compound No. 5311

Compound Name **2-Methylpentanal**

Molecular Formula C6H12O

Molecular weight 100.1600

CAS No 123-15-9

Beil/n20 = 1.401

E = **0.135**

C_w= 0.000

C_g= 0.000

log Kw= #DIV/0!

P + L, count: 8

WS (mg/L)=

VP (mm Hg)=

P+L, sd: **0.061**

Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)
	1.892	1.892	1.30	1.78

P+L, sd(W): **0.061**

Acetaldeh	UNIX	SMART			PA
0.208	0.26	0.135	logKw	1.567	
0.670	0.59	0.60	R (**E**)=	**0.135**	0.24
0.000	0.00	0.00	Pi (**S**)=	0.520	0.72
0.450	0.45	0.40	Alpha (**A**) =	**0.000**	0.00
1.230	3.17	3.267 (L57)	Beta (**B**)=	0.410	0.36
			LogL16 (**L**) =	3.168	3.456
			Vx (**V**)=	0.9697	

P, count: 2

P, sd: **0.015**

L, count: 6

L, sd: **0.072**

											LogPcalc	LogPobs		
											1.724	1.729		
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)	1.896	1.896	1.892	0.000	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	1.552	1.552	1.567	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	3.475	3.475	3.459	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	1.565	1.565	1.567	0.000	
Atmos.Chem.Phys.	DB-5	0.565	-0.099	1.062	0.960	0.000	2.024	0.000	RI/100	DB-5	7.516	7.516	7.458	0.003	
JAFC (1976) 24(2)	OV-1	0.422	0.000	0.672	1.155	0.000	2.067	0.000	RI/100	OV-1	7.320	7.320	7.400	0.006	
Composition and D	DB-1	0.569	-0.446	1.091	1.756	-0.349	2.025	0.000	RI/100	DB-1	7.348	7.348	7.251	0.009	
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	7.369	7.369	7.450	0.007	
Eur J Lipid Sci Tec	RTX-5	0.630	-0.363	1.482	1.492	-0.374	2.006	0.000	RI/100	RTX-5	7.553	na		na	7.030