SMILES	c1(sccc1C)C=O			C_w=	
Compound No.	20515			C_g=	
Compound Name	**2-formyl-3-methylthiophene**			**log Kw=**	
Molecular Formula	C6H6OS			P + L, count:	11
Molecular weight	126.1800	**WS (mg/L)=**			
CAS No	5834-16-2	**VP (mm Hg)=**		**P+L, sd:**	**0.119**
S-A/n20 =	1.587				
E =	1.022			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.815		1.68	1.48	**P+L, sd(W):**	**0.119**

UNIX	**SMART**			**PA**		
0.89		logKw	3.336		P, count:	3
0.93		R (**E**)=	**1.022**	**0.78**		
0.00		Pi (**S**)=	1.230	**1.05**	**P, sd:**	**0.119**
0.50		Alpha (**A**) =	**0.000**	**0.00**		
4.44		Beta (**B**)=	0.310	**0.34**	L, count:	8
		LogL16 (**L**) =	4.632	**4.526**		
		Vx (**V**)=	0.9386		**L, sd:**	**0.128**

LogPcalc	LogPobs
2.240	2.149

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)	1.873	1.873	1.815	0.003	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.431	1.431	1.296	0.018	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.416	3.416	3.336	0.006	

											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	5.093	5.093	5.151	0.003	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	4.632	4.632	4.632	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.449	3.449	3.336	0.013	
J Braz Chem Soc (	DB-5	0.729	0.385	0.000	0.000	1.209	2.004	0.000	RI/100	DB-5	10.780	na		na	11.210
J Braz Chem Soc (	CP-Wax	-0.109	1.004	6.749	9.953	0.000	1.914	0.000	RI/100	CP-Wax	18.084	18.084	18.150	0.004	
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	11.069	11.069	11.090	0.000	
JAFC (2002) 50(5)	BPX-5	0.411	0.000	1.247	1.297	0.169	2.033	0.000	RI/100	BPX-5	11.414	11.414	11.260	0.024	
JAFC (1991) 39(4)	DB-1	0.541	0.000	0.691	0.900	0.164	2.009	0.000	RI/100	DB-1	10.747	10.747	10.920	0.030	
JAFC (1989) 37(4)	DB-1	0.419	-0.299	0.763	1.567	0.000	2.072	0.000	RI/100	DB-1	10.649	10.649	10.450	0.040	