SMILES	C(CC=O)SC					
Compund No.						
Compund Name	**Methional**					
Molecular Formula	C4H8OS				P + L, count:	11
Molecular weight	104.1717					
CAS No	3268-49-3				**P+L, sd:**	**0.059**
S-A/n20 =	1.483					
E =	**0.546**				Weight:	1.00
		MD	**PA**	**ACD**		
ClogP		0.420	0.06	0.71	**P+L, sd(W):**	**0.059**

UNIX	**SMART**			**PA**		
		logKw	4.157		P, count:	2
0.60		R (**E**)=	**0.546**	**0.47**		
0.82		Pi (**S**)=	0.940	**0.94**	**P, sd:**	**0.054**
0.00		Alpha (**A**) =	**0.000**	**0.00**		
0.60		Beta (**B**)=	0.660	**0.68**	L, count:	9
3.66		LogL16 (**L**) =	3.680	**3.759**		
		Vx (**V**)=	**0.8514**		**L, sd:**	**0.063**

											LogPcalc	LogPobs		
											2.270	2.289		
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)	0.368	0.368	0.420	0.003	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.172	4.172	4.157	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	4.570	4.570	4.577	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.150	4.150	4.157	0.000
JCA (2000) 896 36	DB-Wax	-0.320	0.964	6.177	9.496	0.000	2.109	0.000	RI/100	DB-Wax	13.774	na		na
JFAC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	9.166	9.166	9.280	0.013
JAFC (1999) 47(12	CPWax-52CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CPWax-52CB	13.537	na		na
JAFC (2000) 48(2)	DB-Wax	-1.307	0.523	9.055	10.206	0.000	1.977	0.000	RI/100	DB-Wax	14.766	14.766	14.740	0.001
JAFC (2001) 49(6)	DB-Wax	-2.488	0.000	8.261	11.077	2.463	2.106	0.000	RI/100	DB-Wax	14.653	14.653	14.690	0.001
JAFC (2002) 50(8)	2385-2391	0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100		8.711	8.711	8.660	0.003
JAFC (2005) 53(8)	DB5-MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB5-MS	9.493	na		na
Food Chem (2003)	HP-1	0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100	HP-1	8.632	8.632	8.620	0.000
Food Res Int (2001	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	9.038	9.038	9.080	0.002
JAFC (2000) 48(2)	DB-5	-0.139	-1.242	2.721	2.102	0.000	2.016	0.000	RI/100	DB-5	9.159	9.159	9.050	0.012