SMILES	CSSSC			C_w=	
Compound No.	77891			C_g=	
Compound Name	**Dimethyl trisulfide**			**log Kw=**	
Molecular Formula	C2H6S3			P + L, count:	18
Molecular weight	126.2670	**WS (mg/L)=**			
CAS No	3658-80-8	**/P (mm Hg)=**		**P+L, sd:**	**0.078**
S-A/n20 =	1.602				
E =	**1.053**			Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	2.170		1.57	2.93	**P+L, sd(W):** **0.078**

UNIX	**SMART**			**PA**		
		logKw	2.206		P, count:	3
1.13	1.000	R (**E**)=	**1.053**	1.04		
0.70		Pi (**S**)=	0.670	0.63	**P, sd:**	**0.031**
0.00	0.00	Alpha (**A**) =	**0.000**	0.00		
0.60		Beta (**B**)=	0.340	0.41	L, count:	15
4.54	4.630	LogL16 (**L**) =	4.203	4.428		
		Vx (**V**)=	0.8809		**L, sd:**	**0.085**

											LogPcalc	LogPobs	
											2.105	2.124	
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)	2.157	2.157	2.170	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.956	1.956	1.997	0.002
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.202	2.202	2.206	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	4.371	4.371	4.376	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	4.203	4.203	4.203	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.174	2.174	2.206	0.001	
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	9.835	9.835	9.820	0.000	
JSFA (2004) 84 82	CP-SIL-8CB	0.490	0.000	0.962	0.863	0.259	2.030	0.000	RI/100	CP-SIL-8CB	9.755	9.755	9.710	0.002	
JCA (2000) 905 23	CP-SIL-8CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-SIL-8CB	9.653	9.653	9.820	0.028	
Food Chem. (2004)	CP-SIL-8CB	0.532	-0.473	1.552	1.340	-0.344	2.030	0.000	RI/100	CP-SIL-8CB	9.489	na		na	9.840
JAFC (2005) 53(7)	2616-2622	-0.392	1.168	5.931	9.269	0.477	2.056	0.000	RI/100		13.616	13.616	13.750	0.018	
JAFC (1994) 42(3)	DB-1	0.497	0.000	0.738	0.967	0.000	2.018	0.000	RI/100	DB-1	9.474	9.474	9.410	0.004	
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	9.913	9.913	9.940	0.001	
JAFC (1999) 47(12	CPWax-52CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CPWax-52CB	13.644	13.644	13.590	0.003	
JAFC (1999) 47(12	CP-SIL-8CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CP-SIL-8CB	9.566	9.566	9.630	0.004	
JAFC (2002) 50(2)	DB-Wax	-0.659	0.000	6.957	10.472	0.000	2.129	0.000	RI/100	DB-Wax	12.951	na		na	13.600
JAFC (2005) 53(8)	DB-5MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB-5MS	9.142	na		na	9.730
Food Chem. (2003)	HP1	0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100	HP1	9.294	na		na	9.530
Talanta (2003) 60 7	BPX-5	0.747	-0.452	1.223	1.642	0.000	1.977	0.000	RI/100	BPX-5	9.400	na		na	9.770
JAFC (1989) 37(3)	Basic	0.306	0.000	0.789	0.918	0.000	2.069	0.000	RI/100	Basic	9.531	9.531	9.400	0.017	
JAFC (1989) 37(3)	Acidic	0.236	0.720	0.546	0.881	0.342	1.962	0.000	RI/100	Acidic	9.723	na		na	9.410
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	9.477	9.477	9.410	0.004	
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	9.803	9.803	9.900	0.009	
"Quant Analysis Fla	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	9.967	na		na	9.520
"Quant Analysis Fla	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	14.091	14.091	14.000	0.008	