SMILES	CSSCC			C_w=	
Compound No.	77621			C_g=	
Compound Name	**Methyl ethyl disulfide**			**log Kw=**	
Molecular Formula	C3H8S2			P + L, count:	12
Molecular weight	108.2300	**WS (mg/L)=**			
CAS No	20333-39-5	**VP (mm Hg)=**		**P+L, sd:**	**0.042**
ACD/n20 =	1.514				
E =	0.679			Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	2.271		2.76	2.30	**P+L, sd(W):** **0.042**

UNIX	**SMART**			**PA**		
0.80		logKw	1.399		P, count:	3
0.51		R (**E**)=	0.690	**0.69**		
0.00		Pi (**S**)=	0.600	**0.48**	**P, sd:**	**0.022**
0.43		Alpha (**A**) =	**0.000**	**0.00**		
3.78		Beta (**B**)=	0.250	**0.29**	L, count:	9
		LogL16 (**L**) =	3.587	**3.697**		
		Vx (**V**)=	0.8583		**L, sd:**	**0.048**

											LogPcalc	LogPobs		
											1.938	1.953		
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)	2.252	2.252	2.271	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.165	2.165	2.189	0.001	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	1.398	1.398	1.399	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	3.664	3.664	3.670	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.587	3.587	3.587	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	1.381	1.381	1.399	0.000
J Anal Chem USSF	Apiezone	0.611	0.923	0.420	1.369	0.000	1.949	0.000	RI/100	Apiezone	8.491	8.491	8.530	0.001
J Anal Chem USSF	OV-17	0.689	1.376	1.471	0.000	0.297	1.972	0.000	RI/100	OV-17	9.669	9.669	9.740	0.005
J Anal Chem USSF	Triton X-305	0.871	1.452	3.776	5.774	0.000	1.944	0.000	RI/100	Triton X-305	11.112	11.112	11.120	0.000
J Anal Chem USSF	PEG-1000	1.610	2.583	2.789	9.044	-0.713	1.945	0.000	RI/100	PEG-1000	11.865	11.865	11.900	0.001
German Thesis	DB-1	0.592	0.000	0.627	1.106	0.000	2.018	0.000	RI/100	DB-1	8.207	8.207	8.150	0.003
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	8.543	8.543	8.460	0.007