SMILES	S(CC=C)SC			C_w=	
Compound No.	77852			C_g=	
Compound Name	**Allyl methyl disulfide**			**log Kw=**	
Molecular Formula	C4H8S2			P + L, count:	14
Molecular weight	120.2400	**WS (mg/L)=**			
CAS No	2179-58-0	**VP (mm Hg)=**		**P+L, sd:**	**0.074**
ACD/n20 =	1.529				
E =	0.767			Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	2.516		3.01	2.60	**P+L, sd(W):** **0.074**

UNIX	**SMART**			**PA**		
0.93		logKw	1.565		P, count:	3
0.55		R (**E**)=	0.780	**0.81**		
0.00		Pi (**S**)=	0.700	**0.54**	**P, sd:**	**0.094**
0.45		Alpha (**A**) =	**0.000**	**0.00**		
4.17		Beta (**B**)=	0.250	**0.34**	L, count:	11
		LogL16 (**L**) =	3.955	**4.132**		
		Vx (**V**)=	0.9562		**L, sd:**	**0.074**

LogPcalc	LogPobs
2.229	2.157

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)	2.571	2.571	2.516	0.003	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.498	2.498	2.390	0.012	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	1.619	1.619	1.565	0.003	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	logL(calc)	logL(calc)	logL(obs)	(Po-Pc)^2
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	4.050	4.050	4.081	0.001
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.955	3.955	3.955	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	1.650	1.650	1.565	0.007
J Anal Chem USSF	Apiezone	0.611	0.923	0.420	1.369	0.000	1.949	0.000	RI/100	Apiezone	9.333	9.333	9.280	0.003
J Anal Chem USSF	OV-17	0.689	1.376	1.471	0.000	0.297	1.972	0.000	RI/100	OV-17	10.665	10.665	10.640	0.001
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	12.335	12.335	12.290	0.002
J Anal Chem USSF	PEG-1000	1.610	2.583	2.789	9.044	-0.713	1.945	0.000	RI/100	PEG-1000	13.091	13.091	13.220	0.017
Meat Sci (1996) 44	DB-5	0.493	-0.430	1.327	1.408	0.000	2.048	0.000	RI/100	DB-5	9.186	9.186	9.280	0.009
JAFC (1976) 24(2)	OV-1	0.422	0.000	0.672	1.155	0.000	2.067	0.000	RI/100	OV-1	9.067	9.067	8.950	0.014
JAFC (2000) 48(6)	HP-5	0.307	-0.424	1.298	1.348	0.000	2.088	0.000	RI/100	HP-5	9.142	9.142	9.120	0.001
Food Res Int (2001	HP-5MS	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	HP-5MS	9.164	9.164	9.130	0.001