SMILES	C(CSC)=C			C_w=	
Compound No.	**76852**			C_g=	
Compound Name	**Allyl methyl sulfide**			**log Kw=**	
Molecular Formula	C4H8S			P + L, count:	11
Molecular weight	88.1700	**WS (mg/L)=**			
CAS No	10152-76-8	**VP (mm Hg)=**		**P+L, sd:**	**0.025**
S-A/n20 =	1.471				
E =	0.496			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.620	1.616	1.58	1.68	**P+L, sd(W):**	**0.025**

UNIX	**SMART**			**PA**		
0.60		logKw	1.592		P, count:	3
0.36		R (**E**)=	**0.496**	**0.47**		
0.00		Pi (**S**)=	0.500	**0.39**	**P, sd:**	**0.030**
0.28		Alpha (**A**) =	**0.000**	**0.00**		
2.91		Beta (**B**)=	0.360	**0.21**	L, count:	8
		LogL16 (**L**) =	2.932	**2.906**		
		Vx (**V**)=	0.7927		**L, sd:**	**0.025**

LogPcalc	LogPobs
1.536	1.517

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)	1.618	1.618	1.620	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.371	1.371	1.341	0.001	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	1.621	1.621	1.592	0.001	

											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	3.188	3.188	3.212	0.001	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	2.932	2.932	2.932	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	1.617	1.617	1.592	0.001	
J Anal Chem USSF	Apiezone	0.611	0.923	0.420	1.369	0.000	1.949	0.000	RI/100	Apiezone	6.994	6.994	6.970	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	7.996	7.996	7.990	0.000	
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	9.179	9.179	9.210	0.001	
J Anal Chem USSF	PEG-1000	1.610	2.583	2.789	9.044	-0.713	1.945	0.000	RI/100	PEG-1000	9.732	na		na	10.010
JAFC (1976) 24(2)	OV-1	0.422	0.000	0.672	1.155	0.000	2.067	0.000	RI/100	OV-1	6.819	6.819	6.780	0.002	
Meat Sci (1996) 44	DB-5	0.493	-0.430	1.327	1.408	0.000	2.048	0.000	RI/100	DB-5	6.948	6.948	6.960	0.000	