SMILES	CCCSCC=C			C_w=	
Compound No.	**76854**			C_g=	
Compound Name	**Allyl propyl sulfide**			**log Kw=**	
Molecular Formula	C6H12S			P + L, count:	11
Molecular weight	116.2300	**WS (mg/L)=**			
CAS No	27817-67-0	**VP (mm Hg)=**		**P+L, sd:**	**0.064**
ACD/n20 =	1.462				
E =	0.437			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	2.674		2.55	2.60	**P+L, sd(W):**	**0.064**

UNIX	**SMART**			**PA**		
0.60	0.47est	logKw	1.310		P, count:	3
0.36	0.43 est	R (**E**)=	0.500	**0.47**		
0.00	0.00	Pi (**S**)=	0.470	**0.40**	**P, sd:**	**0.074**
0.28	0.375 est	Alpha (**A**) =	**0.000**	**0.00**		
3.91	3.93 est	Beta (**B**)=	0.370	**0.22**	L, count:	8
		LogL16 (**L**) =	3.837	**3.895**		
		Vx (**V**)=	1.0745		**L, sd:**	**0.066**

											LogPcalc	LogPobs		
											2.221	2.170		
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)	2.692	2.692	2.674	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.622	2.622	2.527	0.009	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	1.350	1.350	1.310	0.002	

											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	3.957	3.957	3.984	0.001
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.837	3.837	3.837	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	1.393	1.393	1.310	0.007
J Anal Chem USSF	Apiezone	0.611	0.923	0.420	1.369	0.000	1.949	0.000	RI/100	Apiezone	8.748	8.748	8.700	0.002
J Anal Chem USSF	OV-17	0.689	1.376	1.471	0.000	0.297	1.972	0.000	RI/100	OV-17	9.745	9.745	9.730	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	10.831	10.831	10.810	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	11.411	11.411	11.520	0.012
JAFC (1976) 24(2)	OV-1	0.422	0.000	0.672	1.155	0.000	2.067	0.000	RI/100	OV-1	8.669	8.669	8.580	0.008