SMILES	C(C=C)C#N		C_w= 0.502
Compound No.	6671		C_g= 0.001
Compound Name	**Allyl cyanide**		**log Kw=** 2.703
Molecular Formula	C4H5N		P + L, count: 10
Molecular weight	67.0900	**WS (mg/L)=** 33700.000	
CAS No	109-75-1	**VP (mm Hg)= 18.500**	**P+L, sd: 0.051**
S-A/n20 =	1.406		
E =	**0.284**		Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)	
0.400	0.380	0.380	0.40	0.40	**P+L, sd(W): 0.051**

UNIX	SMART			PA	
		logKw	2.746		P, count: 2
0.41	0.284	R (**E**)=	**0.284**	0.31	
0.97	0.89	Pi (**S**)=	0.810	0.79	**P, sd: 0.043**
0.02	0.00	Alpha (**A**) =	**0.000**	0.00	
0.38	0.39	Beta (**B**)=	0.430	0.26	L, count: 8
2.42		LogL16 (**L**) =	2.536	2.402	
		Vx (**V**)=	0.6430		**L, sd: 0.055**

LogPcalc	LogPobs
1.558	1.573

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)	0.358	0.358	0.400	0.002	P^*
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.757	2.757	2.746	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	3.167	3.167	3.146	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.714	2.714	2.746	0.001
JCA (1995) 708 28	BPX-5 (25m)	0.861	-0.321	1.347	-4.545	0.000	1.932	0.000	RI/100	BPX-5 (25m)	6.760	6.760	6.800	0.002
J Chromatog (1989	PoraPLOT-Q (100C)	0.928	-1.438	0.000	1.802	1.412	1.927	0.000	RI/100	PoraPLOT-Q (100C)	6.013	6.013	6.110	0.009
J Chromatog (1989	PoraPLOT-Q (160C)	1.118	-1.096	0.000	0.000	1.541	1.833	0.000	RI/100	PoraPLOT-Q (160C)	6.117	6.117	6.058	0.004
JCA (1995) 708 28	BPX-5 (12m)	0.911	-0.317	1.261	-4.295	0.000	1.917	0.000	RI/100	BPX-5 (12m)	6.703	6.703	6.730	0.001
JAFC (2002) 50(22	HP-5MS	0.691	-0.352	1.227	1.125	0.000	1.989	0.000	RI/100	HP-5MS	6.628	6.628	6.580	0.002
JCA (2002) 974 16	DB-5	0.738	0.000	1.299	1.585	0.000	1.907	0.000	RI/100	DB-5	6.626	6.626	6.580	0.002