SMILES	CC(=C)C#N		C_w= **0.379**
Compound No.	6662		C_g= 0.004
Compound Name	**Methacrylonitrile**		**log Kw=** 1.995
Molecular Formula	C4H5N		P + L, count: 9
Molecular weight	67.0892	**WS (mg/L)=** 25400	
CAS No	126-98-7	**VP (mm Hg)=** 71.2	**P+L, sd: 0.054**
S-A/n20 =	1.400		
E =	**0.263**		Weight: 1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
0.680	0.600	0.600	0.59	0.74	**P+L, sd(W): 0.054**

UNIX	**SMART**			**PA**	
0.42	0.264	logKw	**1.995**		P, count: 3
0.65	0.53	R (**E**)=	**0.263**	0.29	
0.00	0.00	Pi (**S**)=	0.650	0.73	**P, sd: 0.056**
0.24	0.40	Alpha (**A**) =	**0.000**	0.00	
2.37		Beta (**B**)=	0.360	0.27	L, count: 6
		LogL16 (**L**) =	2.321	2.266	
		Vx (**V**)=	**0.6430**		**L, sd: 0.059**

LogPcalc	LogPobs
1.022	1.000

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)	0.758	0.758	0.680	0.006
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	0.309	0.309	0.326	0.000
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	1.999	1.999	1.995	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	2.769	2.769	2.675	0.009
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	1.967	1.967	1.995	0.001
J Chromatog (198	OnPoraPLOTQ	0.928	-1.438	0.000	1.802	1.412	1.927	0.000	RI/100	OnPoraPLOTQ	5.530	5.530	5.605	0.006
J Chromatog (198	OnPoraPLOTQ	1.118	-1.096	0.000	0.000	1.541	1.833	0.000	RI/100	OnPoraPLOTQ	5.638	5.638	5.596	0.002
JCA (1995) 708 28	BPX5	0.861	-0.321	1.347	-4.545	0.000	1.932	0.000	RI/100	BPX5	6.136	6.136	6.140	0.000
JCA (1995) 708 28	BPX5	0.911	-0.317	1.261	-4.295	0.000	1.917	0.000	RI/100	BPX5	6.096	6.096	6.110	0.000
Restek Data	Rtx-624	-8.632	-4.150	9.487	10.915	0.000	8.817	0.000	RT	Rtx-624	16.904	na		na
Restek Data	Rtx-1	-15.123	0.000	3.717	4.015	0.000	11.350	0.000	RT	Rtx-1	13.632	na		na
Restek Data	Rtx-502.2	-16.261	0.000	9.400	5.769	0.000	11.586	0.000	RT	Rtx-502.2	16.735	na		na