SMILES	c1sc(nc1)C(C)=O			C_w=	
Compound No.	20615			C_g=	
Compound Name	**2-Acetylthiazole**			**log Kw=**	
Molecular Formula	C5H5NOS			P + L, count:	18
Molecular weight	127.1650	**WS (mg/L)=**			
CAS No	24295-03-2	**VP (mm Hg)=**		**P+L, sd:**	**0.060**
S-A/n20 =	1.548				
E =	**0.834**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	0.700		0.80	0.37	**P+L, sd(W):**	**0.060**

UNIX	**SMART**					
0.92	0.834	logKw	4.429	PA	P, count:	3
		R (**E**)=	**0.834**	0.85		
1.19		Pi (**S**)=	1.130	1.32	**P, sd:**	**0.077**
0.00	0.00	Alpha (**A**) =	0.000	0.00		
0.64		Beta (**B**)=	0.600	0.60	L, count:	15
4.75		LogL16 (**L**) =	4.215	4.588		
		Vx (**V**)=	0.8975		**L, sd:**	**0.060**

LogPcalc	LogPobs
1.693	1.638

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)	0.713	0.713	0.700	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.127	-0.127	-0.215	0.008
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.492	4.492	4.429	0.004

											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	5.078	5.078	5.129	0.003	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	4.215	4.215	4.215	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.505	4.505	4.429	0.006	
Flav Frag J (2002)	SPB-5	0.552	-0.435	1.225	1.251	0.000	2.049	0.000	RI/100	SPB-5	10.209	10.209	10.140	0.005	
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	10.382	10.382	10.400	0.000	
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	10.369	10.369	10.380	0.000	
JAFC (1994) 42(3)	DB-1	0.497	0.000	0.738	0.967	0.000	2.018	0.000	RI/100	DB-1	9.836	9.836	9.790	0.002	
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	9.798	9.798	9.730	0.005	
JAFC (1998) 46(2)	InnoWax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	InnoWax	16.248	16.248	16.230	0.000	
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	10.242	10.242	10.360	0.014	
JAFC (2002) 50(2)	DB-Wax	-0.659	0.000	6.957	10.472	0.000	2.129	0.000	RI/100	DB-Wax	16.175	na		na	14.040
Food Chem. (2003)	HP-1	0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100	HP-1	9.802	9.802	9.760	0.002	
JCA (2000) 905 23	CP-SIL-8CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-SIL-8CB	10.321	10.321	10.270	0.003	
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	10.395	10.395	10.350	0.002	
Final Report March	DB-5	1.154	0.000	0.000	0.000	1.423	1.922	0.000	RI/100	DB-5	10.108	10.108	10.150	0.002	
"Quant Anal Flav F	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	16.308	16.308	16.390	0.007	
"Quant Anal Flav F	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	10.406	na		na	9.950