SMILES N(=C(/C)C)\O

Compound No.

Compound Name **Acetone oxime**

Molecular Formula C3H7NO

Molecular weight 73.0900

CAS No 127-06-0

C_w=

C_g=

log Kw=

P + L, count: 16

P+L, sd: 0.040

Weight: 1.00

P+L, sd(W): 0.040

P, count: 5

P, sd: 0.052

L, count: 11

L, sd: 0.035

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**
0.120	0.120	0.122	0.23	0.12
	N=15, S=0.066			
UNIX	4.514	logKw	4.456	PA
0.50	**0.390**	R (**E**)=	**0.390**	0.38
0.60	0.650	PI (**S**)=	0.660	0.32
0.35	0.370	Alpha (**A**) =	0.370	0.31
0.60	0.569	Beta (**B**)=	0.560	0.46
1.82	2.646	LogL16 (**L**) =	2.557	2.051
	0.6468	Vx (**V**)=	0.6468	

CCl_3/Water

Flask 1-Measure 1 logP= -0.400 (not good measure)
Flask 1-Measure 2 logP= -0.355
Flask 1-Measure 3 logP= -0.297 **AVERAGE** -0.351
Flask 1-Measure 1 logP= **SD** 0.050
Flask 2-Measure 2 logP=
Flask 2-Measure 3 logP=

Toluene/water

Flask 1-Measure 1 logP= -0.920 (not very good measurement)
Flask 1-Measure 2 logP= -0.980
Flask 1-Measure 3 logP= -0.982 **AVERAGE** -0.960
Flask 2-Measure 1 logP= **SD** 0.035
Flask 2-Measure 2 logP=
Flask 2-Measure 3 logP=

Hexane/water

Flask 1-Measure 1 logP= -1.784
Flask 1-Measure 2 logP= -1.669
Flask 1-Measure 3 logP= N/A **AVERAGE** -1.725
Flask 2-Measure 1 logP= -1.751 **SD** 0.048
Flask 2-Measure 2 logP= -1.738
Flask 2-Measure 3 logP= -1.682

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	LogPcalc	LogPcalc	LogPobs	(Po-Pc)^2	
												0.324	0.308		
	Octanol	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814	P	Octanol (wet)	0.153	0.153	0.120	0.001	P*
Jamie	Trichloromethane	0.327	0.157	-0.391	-3.191	-3.437	0.000	4.191	P	Trichloromethane	-0.265	-0.265	-0.351	0.007	
Caroline	Hexane August 98	0.361	0.579	-1.723	-3.599	-4.764	0.000	4.344	P	Hexane August 98	-1.741	-1.741	-1.725	0.000	
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	-1.002	-1.002	-0.960	0.002	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.474	4.474	4.456	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	4.567	4.567	4.576	0.000	
	Chloroform	0.116	-0.467	1.203	0.138	1.432	0.994	0.000	L	CHCl3/Wet/25.8.97	4.123	4.123	4.105	0.000	
Caroline	Hexane	0.292	-0.169	0.000	0.000	0.000	0.979	0.000	L	Hexane	2.729	2.729	2.731	0.000	
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	3.470	3.470	3.496	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.457	4.457	4.456	0.000	
Ricardo	CW-20M	-3.270	0.144	1.420	1.950	0.000	0.467	0.000	logtr'	CW-20M	-0.360	-0.360	-0.287	0.005	
Ricardo	Squalene	-2.220	0.143	0.000	0.000	0.000	0.611	0.000	logtr'	Squalene	-0.602	na		na	-0.368
Javi	OV-275	-2.822	0.355	1.650	1.797	0.325	0.341	0.000	logtr'	OV-275	0.125	0.125	0.058	0.004	
Javi	HP-Innowax	-2.675	0.033	1.290	1.703	-0.051	0.386	0.000	logtr'	HP-Innowax	-0.222	-0.222	-0.227	0.000	
Javi	DEGS	-3.296	0.327	1.568	1.882	0.297	0.424	0.000	logtr'	DEGS	-0.186	-0.186	-0.152	0.001	
	Porapak Q	1.547	-0.694	0.000	0.000	0.386	1.756	0.000	I/100	Porapak Q	5.983	5.983	5.980	0.000	5.980
	Book 90	0.838	-0.197	0.635	1.184	0.119	1.969	0.000	I/100	Book90	6.719	6.719	6.700	0.000	6.700