SMILES C1/C(CCCC1)=N/O

Compound No.

Compound Name **Cyclohexanone, oxime**

Molecular Formula C6H11NO

Molecular weight 113.1600

CAS No 100-64-1

ACD/n20 = 1.529

E = 0.768

WS (mg/L)= 18000

VP (mm Hg)=

C_w= 0.159

C_g= 0.000

log Kw= #DIV/0!

P + L, count: 53

P+L, sd: 0.063

Weight: 1.00

P+L, sd(W): 0.063

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**
0.840	1.195	1.195	1.19	1.12

UNIX **SMART**

logKw	5.115	PA	
R (**E**)=	**0.580**	0.58	
PI (**S**)=	0.900	0.42	
Alpha (**A**) =	0.330	0.31	
Beta (**B**)=	0.610	0.45	
LogL16 (**L**) =	4.320	3.823	
Vx (**V**)=	0.9609		

P, count: 5

P, sd: 0.121

L, count: 48

L, sd: 0.057

Octanol/water

Meas. 1 (CW-20M	0.988		
Meas. 2 (CW-20M	0.479*	*Bad measurement	
Meas. 3 (CW-20M	0.936		

Chloroform/water

Meas. 1 (CW-20M	0.818	**Average**	0.821
Meas. 2 (CW-20M	0.839	**sd**	0.017
Meas. 3 (CW-20M	0.805		

Hexane/water

Meas. 1 (CW-20M	-0.630	**Average**	-0.599
Meas. 2 (CW-20M	-0.570	**sd**	0.030
Meas. 3 (CW-20M	-0.596		

Toluene/water

Meas. 1 (CW-20M	**0.260**		
Meas. 2 (CW-20M	0.478*	*Bad measurement	
Meas. 3 (CW-20M	0.150		
Meas. 4 (CW-20M	0.290	**Average**	0.210
Meas. 5 (CW-20M	0.140	**sd**	0.076

											LogPcalc	LogPobs	
											1.289	1.317	
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)	1.031	1.031	0.988	0.002
Jamie	Trichloromethane	0.327	0.157	-0.391	-3.191	-3.437	0.000	4.191	P	Trichloromethane	0.944	0.944	0.821	0.015
Caroline	Hexane August 98	0.361	0.579	-1.723	-3.599	-4.764	0.000	4.344	P	Hexane August 98	-0.773	-0.773	-0.599	0.030
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.011	5.011	5.115	0.011
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	0.232	0.232	0.260	0.001

											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	6.181	6.181	6.103	0.006	
	Chloroform	0.116	-0.467	1.203	0.138	1.432	0.994	0.000	L	CHCl3/Wet/25.8.97	6.141	6.141	5.936	0.042	
Caroline	Hexane	0.292	-0.169	0.000	0.000	0.000	0.979	0.000	L	Hexane	4.423	4.423	4.516	0.009	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.979	4.979	5.115	0.018	
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	5.423	5.423	5.375	0.002	
Ricardo	CW-20M	-3.270	0.144	1.420	1.950	0.000	0.467	0.000	logtr'	CW-20M	0.752	0.752	0.824	0.005	
Ricardo	Squalene	-2.220	0.143	0.000	0.000	0.000	0.611	0.000	logtr'	Squalene	0.502	na		na	0.869
Javi	OV-275	-2.822	0.355	1.650	1.797	0.325	0.341	0.000	logtr'	OV-275	1.133	1.133	1.106	0.001	
Javi	HP-Innowax	-2.675	0.033	1.290	1.703	-0.051	0.386	0.000	logtr'	HP-Innowax	0.704	0.704	0.765	0.004	
Javi	DEGS	-3.296	0.327	1.568	1.882	0.297	0.424	0.000	logtr'	DEGS	0.939	0.939	0.964	0.001	
HP-5	60	-1.867	-0.088	0.403	0.379	0.000	0.706	0.000	logkobs	HP-5	1.620	na		na	
	80	-1.927	-0.051	0.360	0.303	0.000	0.636	0.000	logkobs		1.215	1.215	1.258	0.002	
	100	-1.970	-0.022	0.329	0.243	0.000	0.573	0.000	logkobs		0.869	0.869	0.916	0.002	
	120	-2.008	0.000	0.305	0.200	0.000	0.518	0.000	logkobs		0.570	0.570	0.613	0.002	
	140	-2.041	0.028	0.274	0.166	0.000	0.471	0.000	logkobs		0.311	na		na	
	160	-2.552	0.050	0.229	0.145	0.000	0.389	0.000	logkobs		-0.589	-0.589	-0.557	0.001	
SPD-Octyl	60	-2.570	0.127	0.066	0.053	0.000	0.774	0.000	logkobs	SPD-Octyl	0.924	na		na	
	80	-2.645	0.165	0.062	0.000	0.000	0.703	0.000	logkobs		0.543	0.543	0.600	0.003	
	100	-2.719	0.181	0.057	0.000	0.000	0.644	0.000	logkobs		0.219	0.219	0.267	0.002	
	120	-2.738	0.189	0.076	0.000	0.000	0.578	0.000	logkobs		-0.063	-0.063	-0.016	0.002	
	140	-2.809	0.198	0.082	0.000	0.000	0.534	0.000	logkobs		-0.313	na		na	
	160	-1.980	0.174	0.059	0.000	0.000	0.431	0.000	logkobs		0.036	0.036	0.084	0.002	
	180	-1.996	0.182	0.060	0.000	0.000	0.391	0.000	logkobs		-0.147	-0.147	-0.104	0.002	
	200	-1.965	0.186	0.048	0.000	0.000	0.350	0.000	logkobs		-0.302	-0.302	-0.250	0.003	
	240	-1.979	0.192	0.052	0.000	0.000	0.287	0.000	logkobs		-0.581	-0.581	-0.530	0.003	
RTX-440	60	-2.353	-0.088	0.555	0.480	0.000	0.731	0.000	logkobs	RTX-440	1.412	na		na	
	80	-2.452	-0.038	0.505	0.389	0.000	0.667	0.000	logkobs		0.990	0.990	1.001	0.000	
	100	-2.537	0.000	0.461	0.316	0.000	0.613	0.000	logkobs		0.630	0.630	0.647	0.000	

	120	-2.584	0.021	0.427	0.271	0.000	0.559	0.000	logkobs		0.317	0.317	0.337	0.000
	140	-2.643	0.038	0.398	0.230	0.000	0.514	0.000	logkobs		0.034	na		na
	160	-2.419	0.046	0.336	0.211	0.000	0.427	0.000	logkobs		-0.176	-0.176	-0.168	0.000
	180	-2.398	0.048	0.312	0.192	0.000	0.382	0.000	logkobs		-0.376	-0.376	-0.368	0.000
	200	-2.403	0.067	0.288	0.181	0.000	0.346	0.000	logkobs		-0.550	-0.550	-0.549	0.000
	220	-2.479	0.077	0.270	0.174	0.000	0.323	0.000	logkobs		-0.739	-0.739	-0.730	0.000
	240	-2.393	0.098	0.226	0.156	0.000	0.284	0.000	logkobs		-0.854	-0.854	-0.842	0.000
DB-1701	60	-2.724	-0.187	0.900	1.028	0.000	0.705	0.000	logkobs	DB-1701	1.362	na		na
	80	-2.807	-0.158	0.847	0.944	0.000	0.637	0.000	logkobs		0.927	na		na
	100	-2.841	-0.115	0.775	0.794	0.000	0.573	0.000	logkobs		0.527	na		na
	120	-2.863	-0.083	0.707	0.681	0.000	0.518	0.000	logkobs		0.188	na		na
	140	-2.852	-0.047	0.638	0.558	0.000	0.461	0.000	logkobs		-0.129	na		na
	160	-2.119	-0.007	0.553	0.575	0.000	0.409	0.000	logkobs		0.331	0.331	0.238	0.009
	180	-2.078	-0.001	0.511	0.488	0.000	0.362	0.000	logkobs		0.106	0.106	0.024	0.007
	200	-2.083	0.020	0.471	0.419	0.000	0.328	0.000	logkobs		-0.092	-0.092	-0.164	0.005
	220	-2.070	0.039	0.428	0.356	0.000	0.295	0.000	logkobs		-0.270	-0.270	-0.333	0.004
DB-1	60	-1.921	-0.064	0.260	0.365	0.000	0.695	0.000	logkobs	DB-1	1.399	na		na
	80	-1.988	-0.036	0.246	0.275	0.000	0.626	0.000	logkobs		1.008	na		na
	100	-2.019	-0.020	0.231	0.216	0.000	0.562	0.000	logkobs		0.676	na		na
	120	-2.057	0.000	0.215	0.171	0.000	0.508	0.000	logkobs		0.388	na		na
	140	-2.076	0.021	0.206	0.121	0.000	0.456	0.000	logkobs		0.131	na		na
Rxi-50	160	-2.104	0.124	0.592	0.283	0.000	0.390	0.000	logkobs	Rxi-50	0.279	0.279	0.264	0.000
	180	-2.110	0.145	0.536	0.258	0.000	0.352	0.000	logkobs		0.062	0.062	0.059	0.000
	200	-2.118	0.160	0.486	0.250	0.000	0.319	0.000	logkobs		-0.127	-0.127	-0.114	0.000
	220	-2.111	0.169	0.446	0.216	0.000	0.288	0.000	logkobs		-0.296	-0.296	-0.297	0.000
	240	-2.093	0.181	0.402	0.192	0.000	0.259	0.000	logkobs		-0.444	-0.444	-0.446	0.000
	60	-2.127	0.034	0.946	0.474	0.000	0.685	0.000	logkobs		1.860	na		na
	80	-2.192	0.090	0.807	0.398	0.000	0.623	0.000	logkobs		1.409	1.409	1.448	0.001
	100	-2.212	0.119	0.739	0.341	0.000	0.560	0.000	logkobs		1.054	na		na
	120	-2.236	0.117	0.713	0.302	0.000	0.505	0.000	logkobs		0.755	0.755	0.778	0.001
	140	-2.242	0.143	0.648	0.269	0.000	0.455	0.000	logkobs		0.479	0.479	0.504	0.001
Hp-Innowax	160	-2.568	0.215	1.157	1.544	0.000	0.356	0.000	logkobs	Hp-Innowax	0.645	0.645	0.634	0.000
	180	-2.383	0.202	0.998	1.363	0.000	0.299	0.000	logkobs		0.374	0.374	0.367	0.000
	200	-2.350	0.204	0.926	1.198	0.000	0.265	0.000	logkobs		0.142	0.142	0.133	0.000
	220	-2.334	0.209	0.854	1.071	0.000	0.237	0.000	logkobs		-0.067	-0.067	-0.077	0.000
DB-225	160	-2.784	0.055	0.980	0.853	0.000	0.340	0.000	logkobs	DB-225	-0.120	-0.120	-0.210	0.008
	180	-2.833	0.074	0.909	0.776	0.000	0.311	0.000	logkobs		-0.372	-0.372	-0.354	0.000
	200	-2.826	0.091	0.842	0.691	0.000	0.278	0.000	logkobs		-0.586	-0.586	-0.600	0.000
	220	-2.775	0.096	0.754	0.612	0.000	0.251	0.000	logkobs		-0.754	-0.754	-0.731	0.001