SMILES	ClC(F)F	4026.000	C_w= 0.310	
	L= 0.690, direct determination		C_g= 0.390	
Compound Name	**Chlorodifluoromethane**		**log Kw=** -0.100	
Molecular Formula	CHClF2	**WS at 21C**	P + L, count:	15
Molecular weight	86.4700	**WS (mg/L)= 26800**		
CAS No	75-45-6	**/P (mm Hg)= 7250**	**P+L, sd:**	**0.085**
Beil/n20 =	1.267			
E =	0.056		Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
1.080	1.072	1.072	1.09	0.98	**P+L, sd(W):** **0.085**

UNIX	**SMART**			**PA**	
0.05	0.000	logKw	**-0.091**		P, count: 7
0.17	0.25	R (**E**)=	**-0.056**	**-0.11**	
0.21	0.20	PI (**S**)=	0.380	**0.19**	**P, sd:** **0.060**
0.00	0.00	Alpha (**A**) =	0.040	**0.12**	
0.62	0.690	Beta (**B**)=	0.050	**0.00**	L, count: 8
		LogL16 (**L**) =	0.706	**0.588**	
		Vx (**V**)=	0.4073		**L, sd:** **0.106**

Kw		**T = 25.0 ± 0.2 C**
Average	-0.239	(See spreadsheet of explanation log Kw
Average	**-0.091**	(Much precise measurement after 48 h
Toluene/air		**T = 25.0 ± 0.2 C**
Average	**1.301**	(see worksheet for explanation)
Octane/air		**T = 25 ± 0.2 C**
Average	**0.859**	(see worksheet for explanation)
Nitromethane (dry)/air		**T = 25.0 ± 0.2 C**
Average	**1.379**	(see worksheet for explanation)
Propanol (dry)/air		**T = 25.0 ± 0.2 C**
Measurement :	1.097	
Measurement :	1.005	
Measurement :	1.095	
Measurement 4		
From L42		
Average	**1.066**	
SD	0.053	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	LogPcalc	LogPcalc	LogPobs	(Po-Pc)^2	
												0.978	0.962		
	Octanol	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814	P	Octanol (wet)	1.038	1.038	1.080	0.002	P*
Caroline	Octane August 98	0.223	0.642	-1.647	-3.480	-5.067	0.000	4.526	P	Octane August 98	1.012	1.012	0.927	0.007	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.017	-0.017	**-0.091**	0.005	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane	0.854	0.854	**0.797**	0.003	
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	1.329	1.329	1.392	0.004	
MHA/Acree	PrOH/Dry	0.148	0.436	-1.098	0.389	-3.893	0.000	4.036	P	PrOH/Dry/Joelle paper	1.171	1.171	1.157	0.000	
	Nitromethane dry	0.023	-0.091	0.793	-1.463	-4.364	0.000	3.460	P	Nitromethane. Dry	1.462	1.462	1.470	0.000	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	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	0.889	0.889	0.989	0.010	
Caroline	Octane	0.215	-0.049	0.000	0.000	0.000	0.967	0.000	L	Octane	0.901	0.901	**0.836**	0.004	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.028	-0.028	**-0.091**	0.004	
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	1.228	1.228	**1.301**	0.005	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	0.706	0.706	**0.690**	0.000	Direct exp.
	Olive oil	-0.156	-0.254	0.859	1.656	0.000	0.873	0.000	L	Olive oil	0.867	0.867	0.640	0.052	0.64 (J.Chem.Inf.Mod., 2006, 46, 1735)
	Propanol, dry	-0.028	-0.185	0.648	4.022	1.043	0.869	0.000	L	PrOH/Dry/Joelle paper	1.055	1.055	**1.066**	0.000	
	Nitromethane, dry	-0.340	-0.297	2.689	2.193	0.514	0.728	0.000	L	Nitromethane, dry	1.326	1.326	**1.379**	0.003	
	Blood,37	-1.069	0.456	1.083	3.738	2.580	0.376	0.000	logL	Blood,37	-0.139	na		na	Eq (9) in pape -0.097
	Fat,37	-0.052	0.051	0.728	1.783	0.332	0.743	0.000	logL	Fat,37	0.834	na		na	q (11) in pape 0.897

>g
48 h - see spreadsl