SMILES C(CC(F)(F)F)(F)(F)F

Compound No. 66825

Compound Name **1,1,1,3,3,3-Hexafluoropropane**

Molecular Formula C3H2F6

Molecular weight 152.0400

CAS No 690-39-1

Paper/n20 = 1.2324 (at 21C)

E = **-0.341**

C_w= 0.000

C_g= 0.000

log Kw= #DIV/0!

P + L, count: 13

WS (mg/L)=

P (mm Hg)=

P+L, sd: **0.079**

Paper- Fluid Phase Equilibria 122 (1996) 187-206

Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	1.099		2.09	1.14	**P+L, sd(W):**	**0.079**

UNIX	SMART			PA		
-0.45	-0.590	logKw	**-0.943**		P, count:	4
-0.13	0.14	R (**E**)=	**-0.588**	-0.59		
0.00	0.06	Pi (**S**)=	0.120	-0.21	**P, sd:**	**0.076**
0.00	0.06	Alpha (**A**) =	0.130	0.09		
-0.02	0.666	Beta (**B**)=	0.030	0.00	L, count:	9
		LogL16 (**L**) =	0.686	0.284		
		Vx (**V**)=	0.6375		**L, sd:**	**0.084**

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	LogPcalc	LogPcalc	LogPobs	(Po-Pc)^2
												1.341	1.368	
Caroline	Octane August 98	0.223	0.642	-1.647	-3.480	-5.067	0.000	4.526	P	Octane August 98	1.929	1.929	1.883	0.002
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	-0.940	-0.940	**-0.943**	0.000
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	2.108	2.108	2.223	0.013
MHA/Acree	PrOH/Dry	0.148	0.436	-1.098	0.389	-3.893	0.000	4.036	P	PrOH/Dry/Joelle paper	2.267	2.267	2.310	0.002

											logL(calc)	logL(calc)	logL(obs)		
Caroline	Octane	0.215	-0.049	0.000	0.000	0.000	0.967	0.000	L	Octane	0.907	0.907	**0.940**	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	-0.919	-0.919	**-0.943**	0.001	
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	1.122	1.122	**1.280**	0.025	
	Propanol, dry	-0.028	-0.185	0.648	4.022	1.043	0.869	0.000	L	PrOH/Dry/Joelle paper	1.309	1.309	**1.367**	0.003	
Anal Chem (1996)	Bruno -20	0.847	-2.165	-1.186	0.366	1.952	2.322	0.000	I/100	Bruno -20	3.677	3.677	3.671	0.000	
Anal Chem (1996)	Bruno 0	0.872	-2.164	-1.144	0.496	0.588	2.276	0.000	I/100	Bruno 0	3.651	3.651	3.640	0.000	
Anal Chem (1996)	Bruno 20	1.602	-1.863	0.637	-0.492	-2.543	1.498	0.000	I/100	Bruno 20	3.661	3.661	3.621	0.002	
Anal Chem (1996)	Bruno 40	1.557	-1.682	0.151	0.954	-1.581	1.550	0.000	I/100	Bruno 40	3.704	3.704	3.594	0.012	
	Saline, 37	-1.471	0.724	2.604	4.147	4.447	-0.188	0.000	L	Saline, 37	-1.040	-1.040	-1.155	0.013	
	Olive oil	-0.156	-0.254	0.859	1.656	0.000	0.873	0.000	L	Olive oil/2006	0.911	na		na	0.707

Kw		**T = 25.0 ± 0.2 C**
Measurement 1	-0.990	
Measurement 2	-0.941	
Measurement 3	-0.926	
Average	**-0.952**	
SD	0.033	

Octane/air		**T = 25 ± 0.2 C**
Measurement 1	0.889	
Measurement 2	0.916	
Measurement 3	0.992	
Measurement 4	0.963	
Measurement 5		
Average	**0.940**	
SD	0.046	

Toluene/air		**T = 25.0 ± 0.2 C**
Measurement 1		Not reliable
Measurement 2	1.329	
Measurement 3	1.289	
Measurement 4	0.976	Not reliable
Measurement 5	1.234	
Measurement 6	1.267	
Average	**1.280**	(only reliable)

Propanol (dry)/air		**T = 25.0 ± 0.2 C**
Measurement 1	1.069	Not reliable
Measurement 2	1.351	
Measurement 3	1.374	
Measurement 4	1.376	
Average	**1.367**	(only reliable)
SD	0.014	

Octanol (dry)/air		**T = 25.0 ± 0.2 C**
Measurement 1	0.785	
Measurement 2		
Measurement 3		
Measurement 4		
Average		Octanol elutes very late. Since only 1 measurement
SD		

Toluene/water		**T = 20.1 ± 0.2 C**
Measurement 1	1.203	Not reliable
Measurement 2	2.508	
Measurement 3	2.300	
Measurement 4	2.380	
Average	**2.396**	Not included since the equilibrium is not established
SD	0.105	

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