SMILES	c1(ccccc1)CC(=O)O				
Compund No.	16351				
Compund Name	**Phenylacetic acid**				
Molecular Formula	$C_8H_8O_2$			P + L, count:	28
Molecular weight	136.148				
CAS No	103-82-2			**P+L, sd:**	**0.084**
ACD/n20 =	1.552				
E =	0.915			Weight:	1.00
	MD	**PA**	**ACD**		
ClogP	1.414	1.55	1.50	**P+L, sd(W):**	**0.084**

UNIX	**SMART**			PA		
0.880	0.730	logKw	6.470		P, count:	13
0.94	1.01	R (**E**)=	0.730	0.860		
0.59	0.59	Pi (**S**)=	1.08	1.01	**P, sd:**	**0.094**
0.47	0.61	Alpha (**A**) =	0.66	0.63		
5.010	4.933	Beta (**B**)=	0.57	0.55	L, count:	15
		LogL16 (**L**) =	4.962	4.993		
		Vx (**V**)=	**1.0726**		**L, sd:**	**0.077**

											LogPcalc	LogPobs	
											1.070	1.056	
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)	1.501	1.501	**1.450**	0.003
a	Isobutanol	0.249	0.480	-0.639	-0.050	-2.284	0.000	2.758	P	Isobutanol	1.532	1.532	1.430	0.010
b	Pentanol	0.175	0.575	-0.787	0.020	-2.837	0.000	3.249	P	Pentanol	1.625	1.625	1.570	0.003
i	Dichloromethane	0.314	0.001	0.022	-3.238	-4.137	0.000	4.259	P	Dichloromethane	0.411	0.411	0.600	0.036
Jamie	Trichloromethane	0.327	0.157	-0.391	-3.191	-3.437	0.000	4.191	P	Trichloromethane	0.449	0.449	0.420	0.001
Caroline	Heptane August 98	0.325	0.670	-2.061	-3.317	-4.733	0.000	4.543	P	Heptane August 98	-1.427	-1.427	-1.400	0.001
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	6.525	6.525	6.470	0.003
BENZ-1	Benzene	0.142	0.464	-0.588	-3.099	-4.625	0.000	4.491	P	Benzene/Dec/1997 (25celi	-0.019	-0.019	-0.030	0.000
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	-0.112	-0.112	-0.130	0.000
a	Nitrobenzene	-0.181	0.576	0.003	-2.356	-4.420	0.000	4.263	P	Nitrobenzene	0.740	0.740	0.670	0.005
a	Diethyl ether	0.248	0.561	-1.016	-0.226	-4.553	0.000	4.075	P	Diethyl ether/ Wet/2002	1.186	1.186	1.330	0.021
h	Dibutylether/W/2002	0.252	0.677	-1.506	-0.807	-5.249	0.000	4.815	P	Dibutylether/ Wet/2002	0.759	0.759	0.760	0.000
a	PGDP	0.139	0.376	-0.715	-1.034	-4.852	0.000	4.245	P	PGDP/Oct 98	0.746	0.746	0.590	0.024

											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	7.963	7.963	7.920	0.002
	Dichloromethane	0.121	-0.450	1.677	0.404	0.786	0.940	0.000	L	Dichloromethane	6.982	6.982	7.070	0.008
	Chloroform	0.116	-0.467	1.203	0.138	1.432	0.994	0.000	L	CHCl3/Wet/25.8.97	6.914	6.914	6.890	0.001
Caroline	Heptane	0.275	-0.162	0.000	0.000	0.000	0.983	0.000	L	Heptane	5.034	5.034	5.070	0.001
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	6.556	6.556	6.470	0.007
BENZ-1	Benzene	0.107	-0.313	1.053	0.457	0.169	1.020	0.000	L	Benzene/Dec 97	6.475	6.475	6.440	0.001
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	6.358	6.358	6.340	0.000
	Nitrobenzene	-0.273	0.039	1.803	1.231	0.000	0.929	0.000	L	Nitrobenzene	7.125	7.125	7.140	0.000
	Diethyl ether / Wet/200	0.206	-0.169	0.873	3.402	0.000	0.882	0.000	L	Diethyl ether/ Wet /2002	7.647	7.647	7.800	0.024
	Dibutylether/ Wet/2002	0.369	-0.216	0.026	2.626	-0.499	1.124	0.000	L	Dibutyl ether/Wet/2002	7.265	7.265	7.230	0.001
JAFC (2001) 49(6)	DB-Wax	-2.488	0.000	8.261	11.077	2.463	2.106	0.000	RI/100	DB-Wax	25.598	25.598	25.710	0.013
JAFC (2001) 49(10	DB-Wax	-1.301	0.000	7.705	11.075	0.000	2.181	0.000	RI/100	DB-Wax	25.151	na		na
JAFC (2005) 53(8)	DB-5MS	-0.254	-0.571	1.228	1.947	2.407	1.988	0.000	RI/100	DB-5MS	13.177	na		na
JAFC (1998) 46(2) 625-633		0.572	0.000	1.006	1.348	-0.654	2.024	0.000	RI/100		12.218	12.218	12.120	0.010
JAFC (2000) 48(2)	DB-Wax	-1.307	0.523	9.055	10.206	0.000	1.977	0.000	RI/100	DB-Wax	25.399	25.399	25.340	0.003
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	12.296	12.296	12.360	0.004
JAFC (1998) 46(2)	InnoWax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	InnoWax	24.621	na		na
Food Chemistry (1999) 64 3-11		0.045	-0.609	1.664	1.596	-0.555	2.067	0.000	RI/100		12.390	12.390	12.300	0.008