SMILES	CCC/C=C/C=O
Compund No.	5410
Compund Name	**(E)-2-hexenal**
Molecular Formula	C6H10O
Molecular weight	98.1430
CAS No	6728-26-3
S-A/n20 =	1.446
E =	**0.372**

	MD	PA	ACD
ClogP	1.578	1.82	1.58

P + L, count:	14
P+L, sd:	**0.047**
Weight:	1.00
P+L, sd(W):	**0.047**
P, count:	2
P, sd:	**0.025**
L, count:	12
L, sd:	**0.050**

UNIX	SMART			PA
		logKw	2.405	
0.41	0.382	R (**E**)=	**0.372**	0.31
0.73	0.80	Pi (**S**)=	0.75	0.67
0.00	0.00	Alpha (**A**) =	**0.00**	0.01
0.45	0.50	Beta (**B**)=	0.43	0.41
3.34	3.400	LogL16 (**L**) =	3.522	3.546
		Vx (**V**)=	**0.9267**	

LogPcalc	LogPobs
1.981	1.991

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	LogPcalc	LogPcalc	LogPobs	(Po-Pc)^2	
		0.104	-0.201	0.154	0.434	0.848	-0.672	-0.797	Sw	(logSw)/5 Joelle paper	-0.230	na		na	
		0.081	-0.097	0.163	0.391	0.804	-0.226	-0.813	Sw	mp term to be added	-0.242	na		na	
	Octanol	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814	P	Octanol (wet)	1.553	1.553	1.578	0.001	CLOGP
a	Isobutanol	0.249	0.480	-0.639	-0.050	-2.284	0.000	2.758	P	Isobutanol	1.522	na		na	
b	Pentanol	0.175	0.575	-0.787	0.020	-2.837	0.000	3.249	P	Pentanol	1.590	na		na	
b	Hexanol	0.143	0.718	-0.980	0.145	-3.214	0.000	3.403	P	Hexanol	1.447	na		na	
b	Decanol	0.008	0.485	-0.974	0.015	-3.798	0.000	3.945	P	Decanol	1.481	na		na	
b	Olely alcohol	-0.359	-0.270	-0.528	-0.035	-4.042	0.000	4.204	P	Oleyl alcohol	1.302	na		na	
i	Dichloromethane	0.314	0.001	0.022	-3.238	-4.137	0.000	4.259	P	Dichloromethane	2.499	na		na	
Jamie	Trichloromethane	0.327	0.157	-0.391	-3.191	-3.437	0.000	4.191	P	Trichloromethane	2.498	na		na	
CTET-1	Tetrachloromethane	0.260	0.573	-1.254	-3.558	-4.588	0.000	4.589	P	CCl4 Sept 98	1.812	na		na	
c/July 1997	1,2-Dichloroethane	0.227	0.278	-0.167	-2.816	-4.324	0.000	4.205	P	1,2-Dichloroethame	2.243	na		na	
Caroline	Pentane August 98	0.369	0.386	-1.568	-3.535	-5.215	0.000	4.514	P	Pentane August 98	1.277	na		na	
Caroline	Hexane August 98	0.361	0.579	-1.723	-3.599	-4.764	0.000	4.344	P	Hexane August 98	1.261	na		na	
Caroline	Heptane August 98	0.325	0.670	-2.061	-3.317	-4.733	0.000	4.543	P	Heptane August 98	1.203	na		na	
Caroline	Octane August 98	0.223	0.642	-1.647	-3.480	-5.067	0.000	4.526	P	Octane August 98	1.242	na		na	
Caroline	Nonane August 98	0.240	0.619	-1.713	-3.532	-4.921	0.000	4.482	P	Nonane August 98	1.223	na		na	
Caroline	Decane August 98	0.160	0.585	-1.734	-3.435	-5.078	0.000	4.582	P	Decane August 98	1.140	na		na	
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.137	na		na	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	2.409	2.409	2.405	0.000	

CYC-1	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577	P	Cyclohexane/Dec 98	1.314	na	na
c	Isooctane	0.288	0.382	-1.668	-3.639	-5.000	0.000	4.561	P	Isooctane	1.256	na	na
BENZ-1	Benzene	0.142	0.464	-0.588	-3.099	-4.625	0.000	4.491	P	Benzene/Dec/1997 (25celi	2.047	na	na
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	1.937	na	na
PHCL-1	Chlorobenzene	0.040	0.246	-0.462	-3.038	-4.769	0.000	4.640	P	Chlorobenzene	2.034	na	na
AMAL	Bromobenzene	-0.130	0.394	-0.280	-3.331	-4.640	0.000	4.583	P	Bromobenzene	2.058	na	na
AMAL	Iodobenzene	-0.181	0.410	-0.334	-3.300	-4.595	0.000	4.549	P	Iodobenzene	1.961	na	na
a	Nitrobenzene	-0.181	0.576	0.003	-2.356	-4.420	0.000	4.263	P	Nitrobenzene	2.085	na	na
a	Diethyl ether	0.248	0.561	-1.016	-0.226	-4.553	0.000	4.075	P	Diethyl ether/ Wet/2002	1.513	na	na
AMAL	Diisopropylether	0.476	0.434	-0.939	-0.555	-5.185	0.000	4.189	P	Diisopropyl ether/ Wet/ 20(	1.586	na	na
h	Dibutylether/W/2002	0.252	0.677	-1.506	-0.807	-5.249	0.000	4.815	P	Dibutylether/ Wet/2002	1.579	na	na
c	Ethyl acetate	0.253	1.157	-1.397	-0.054	-3.755	0.000	3.726	P	Ethyl acetate	1.474	na	na
a	n-Butyl acetate	-0.468	0.712	-0.397	0.010	-3.743	0.000	3.865	P	n-Butyl acetate	1.471	na	na
a	PGDP	0.139	0.376	-0.715	-1.034	-4.852	0.000	4.245	P	PGDP/Oct 98	1.590	na	na
a	Olive oil May 97	-0.011	0.577	-0.800	-1.470	-4.921	0.000	4.173	P	Olive oil May 97 (37celcius	1.355	na	na
AMAL	Tributylphosphate	0.015	0.804	-0.862	1.389	-4.647	0.000	4.129	P	Tributylphosphate	1.496	na	na
	CS2	0.047	0.686	-0.943	-3.603	-5.818	0.000	4.921	P	CS2/August 99	1.653	na	na
MEOH-1	MeOH/Dry	0.329	0.299	-0.671	0.080	-3.389	0.000	3.512	P	MeOH/Dry/Dec 1997	1.734	na	na
ETOH-1	EtOH/Dry	0.208	0.409	-0.959	0.186	-3.645	0.000	3.928	P	EtOH/Dry/Dec 1997	1.714	na	na
MHA/Acree	PrOH/Dry	0.148	0.436	-1.098	0.389	-3.893	0.000	4.036	P	PrOH/Dry/Joelle paper	1.553	na	na
MHA/Acree	BuOH/Dry	0.152	0.438	-1.177	0.096	-3.919	0.000	4.122	P	BuOH/Dry/March 1999	1.567	na	na
Czech	PeOH/DRy	0.080	0.521	-1.294	0.208	-3.908	0.000	4.208	P	PeOH/Dry/Czech	1.522	na	na
Czech	HexOH/Dry	0.044	0.470	-1.153	0.083	-4.057	0.000	4.249	P	HexOH/Dry/Czech	1.547	na	na
	HeptOH/Dry	-0.026	0.491	-1.258	0.035	-4.155	0.000	4.415	P	HeptOH/Dry/Czech	1.518	na	na
MHA	EGLY/Dry/Sept 1998	-0.313	0.419	-0.409	0.906	-2.558	0.000	2.771	P	EGLY/Dry/Sept 1998	1.004	na	na
OCTD-1	OctOH/Dry/Paper	-0.034	0.490	-1.048	-0.028	-4.229	0.000	4.219	P	OctOH/Dry/Paper (25celci	1.454	na	na
	DecOH/Dry	-0.062	0.754	-1.461	0.063	-4.053	0.000	4.293	P	DecOH/Dry/Czech	1.358	na	na
	isoPrOH/Dry	0.063	0.320	-1.024	0.445	-3.824	0.000	4.067	P	iso-PrOH/Dry/June 1999	1.539	na	na
	t-BuOH	0.197	0.136	-0.916	0.318	-4.031	0.000	4.112	P	tert-BuOH/Dry/2001	1.638	na	na
TFE-1	TFE dry	0.368	-0.505	-0.677	-1.756	-0.325	0.000	3.123	P	TFE. Dry	2.427	na	na
	EtOAc dry	0.358	0.362	-0.449	-0.668	-5.016	0.000	4.155	P	EtOAC/Dry/Oct 99	1.849	na	na
MHA	Acetone/Dry	0.335	0.349	-0.231	-0.411	-4.793	0.000	3.963	P	Acetone/Dry/August 99	1.903	na	na
	Butanone(GSW) dry	0.354	0.003	-0.164	-0.979	-4.706	0.000	4.160	P	Butanone(GSW). Dry	2.064	na	na
MHA	DMF dry	0.105	0.317	0.462	1.154	-4.843	0.000	3.757	P	DMF/Dry/Sept 1998	1.969	na	na
MECN-1	MeCN/Dry	0.413	0.077	0.326	-1.566	-4.391	0.000	3.364	P	MeCN/Dry/June 1999	1.915	na	na
	Nitromethane dry	0.023	-0.091	0.793	-1.463	-4.364	0.000	3.460	P	Nitromethane. Dry	1.914	na	na
	NMP dry	-0.071	0.686	0.455	1.547	-5.068	0.000	3.899	P	NMP/Dry/Sept 98	1.959	na	na
	DMSO dry	-0.231	0.520	0.757	1.799	-4.652	0.000	3.428	P	DMSO. Dry	1.707	na	na
FILOMENA	EG/Heptane	0.336	-0.075	-1.201	-3.786	-2.201	0.000	2.085	P	EG/Hept paper	0.393	na	na
Pt32	DlogP(cyc)	-0.039	-0.254	0.677	3.822	1.445	0.000	-0.832	P	DlogPcyc	0.225	na	na
Pt32	DlogP(alkane)	-0.199	-0.087	0.603	3.550	1.358	0.000	-0.468	P	DlogPalk	0.371	na	na
	water-plant	-0.415	0.596	-0.413	-0.508	-4.096	0.000	3.908	P	water-plant, n=62	1.357	na	na
g	Skin eq9 Best	-5.241	0.437	-0.410	-1.631	-3.286	0.000	2.012	P	Skin-Eq.9	-4.934	na	na
e	BB	-0.024	0.270	-0.810	-0.839	-0.486	0.000	0.965	P	BB-H	0.154	na	na
f	Rat cortex	-1.213	0.771	-1.868	0.000	-2.795	0.000	3.301	P	Saline-cortex-H	-0.470	na	na
f	Rat retina	-1.226	1.358	-1.440	0.000	-2.862	0.000	2.609	P	Saline-retina-H	-0.614	na	na

	Marti/MeOH/HPLC	-0.273	0.364	-0.546	-0.209	-1.225	0.000	1.227	k'	Marti/MeOH/HPLC	0.063	na		na
	Marti/MeCN/HPLC	-0.124	0.231	-0.357	-0.405	-1.016	0.000	0.956	k'	Marti/MeCN/HPLC	0.143	na		na
	HUMAA B-O	-1.718	0.713	0.000	0.000	-2.655	0.000	2.360	k'	HUMAA B-O	-0.407	na		na
	HUMB B-O	-1.132	0.311	0.000	0.000	-2.040	0.000	3.205	k'	HUMB B-O	1.077	na		na
	HUMC B-O	-0.479	0.413	0.000	0.000	-3.084	0.000	3.038	k'	HUMC B-O	1.164	na		na
	HUMO B-O	-0.033	0.529	-0.845	0.000	-3.887	0.000	3.901	k'	HUMO B-O	1.474	na		na
	HUMP B-O	0.842	1.336	-0.833	0.000	-1.771	0.000	1.455	k'	HUMP B-O	1.301	na		na
	SUGB	-0.787	0.407	-0.183	-0.879	-0.615	0.000	0.931	k'	SUGB	-0.175	na		na
	Tom50	-0.669	0.181	-0.687	-0.252	-1.872	0.000	2.491	k'	Tom50	0.387	na		na
	Tom75	-0.919	0.096	-0.479	-0.336	-1.266	0.000	1.617	k'	Tom75	-0.288	na		na
											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	3.971	3.971	3.983	0.000
	Dichloromethane	0.121	-0.450	1.677	0.404	0.786	0.940	0.000	L	Dichloromethane	4.860	na		na
	Chloroform	0.116	-0.467	1.203	0.138	1.432	0.994	0.000	L	CHCl3/Wet/25.8.97	4.961	na		na
CTET-1	Tetrachloromethane	0.282	-0.303	0.460	0.000	0.000	1.047	0.000	L	CCl4/Sept 98	4.202	na		na
	1,2-Dichloroethane	0.011	-0.150	1.436	0.649	0.736	0.936	0.000	L	1,2-DCE/July.97	4.646	na		na
Caroline	Pentane	0.335	-0.276	0.000	0.000	0.000	0.968	0.000	L	Pentane	3.642	na		na
Caroline	Hexane	0.292	-0.169	0.000	0.000	0.000	0.979	0.000	L	Hexane	3.677	na		na
Caroline	Heptane	0.275	-0.162	0.000	0.000	0.000	0.983	0.000	L	Heptane	3.677	na		na
Caroline	Octane	0.215	-0.049	0.000	0.000	0.000	0.967	0.000	L	Octane	3.603	na		na
Caroline	Nonane	0.200	-0.145	0.000	0.000	0.000	0.980	0.000	L	Nonane	3.598	na		na
Caroline	Decane	0.156	-0.143	0.000	0.000	0.000	0.989	0.000	L	Decane	3.586	na		na
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.522	na		na
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	2.412	2.412	2.405	0.000
CYC-1	Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013	0.000	L	Cyclohexane/Dec/98	3.690	na		na
ISOCT-1	Isooctane	0.275	-0.244	0.000	0.000	0.000	0.972	0.000	L	Isooctane	3.608	na		na
BENZ-1	Benzene	0.107	-0.313	1.053	0.457	0.169	1.020	0.000	L	Benzene/Dec 97	4.446	na		na
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	4.349	na		na
PHCL-1	Chlorobenzene	0.053	-0.553	1.254	0.364	0.000	1.041	0.000	L	Chlorobenzene	4.455	na		na
	Nitrobenzene	-0.273	0.039	1.803	1.231	0.000	0.929	0.000	L	Nitrobenzene	4.366	na		na
	Diethyl ether / Wet/200	0.206	-0.169	0.873	3.402	0.000	0.882	0.000	L	Diethyl ether/ Wet /2002	3.905	na		na
	Isopropyl ether Wet/ 2(	0.134	-0.242	0.728	3.191	0.000	0.954	0.000	L	Isopropyl ether /Wet /200	3.950	na		na
	Dibutylether/ Wet/2002	0.369	-0.216	0.026	2.626	-0.499	1.124	0.000	L	Dibutyl ether/Wet/2002	4.053	na		na
	Olive oil	-0.230	0.009	0.795	1.353	0.000	0.888	0.000	L	Olive oil	3.497	na		na
	Ethylhexyl phosphate	-0.090	-0.190	0.830	3.410	0.000	0.890	0.000	L	Ethylhexyl phosphate	3.597	na		na
	CS2	0.101	0.251	0.177	0.027	0.095	1.068	0.000	logL	CS2/August 99	4.130	na		na
MEOH-1	Methanol, dry	-0.004	-0.215	1.173	3.701	1.432	0.769	0.000	L	MeOH/Dry/24.8.97	4.120	na		na
ETOH-1	Ethanol, dry	0.012	-0.206	0.789	3.635	1.311	0.853	0.000	L	EtOH/Dry/24.8.97	4.095	na		na
	Propanol, dry	-0.028	-0.185	0.648	4.022	1.043	0.869	0.000	L	PrOH/Dry/Joelle paper	3.899	na		na
	Butanol, dry	-0.039	-0.276	0.539	3.781	0.995	0.934	0.000	L	BuOH/Dry/March 1999	3.982	na		na
	Pentanol, dry	-0.042	-0.277	0.526	3.779	0.983	0.932	0.000	L	PeOH/Dry/Czech	3.955	na		na
	Hexanol, dry	-0.035	-0.298	0.626	3.726	0.729	0.936	0.000	L	HexOH/Dry/Czech	3.934	na		na

	Heptanol, dry	-0.062	-0.168	0.429	3.541	1.181	0.927	0.000	L	HeptOH/Dry/Czech	3.970	na		na
OCTD-1	Octanol, dry	-0.120	-0.203	0.560	3.576	0.702	0.939	0.000	L	OctOH/Dry/Paper	3.834	na		na
	Decanol, dry	-0.136	-0.038	0.325	3.674	0.767	0.947	0.000	L	DecOH/Dry/Czech	3.759	na		na
	iso-Propanol, dry	-0.060	-0.335	0.702	4.017	1.040	0.893	0.000	L	iso-PrOH/Dry/June 1999	3.935	na		na
	tert-Butanol, dry	0.000	0.000	0.000	0.000	0.000	0.000	0.000	L	tert-BuOH	0.000	na		na
MHA	EGLY, dry	-0.937	0.215	1.511	4.651	2.591	0.571	0.000	L	EGLY/Dry/Sept 1998	3.402	na		na
TFE-1	TFE, dry	-0.133	-0.611	1.457	1.899	4.461	0.633	0.000	L	Trifluroethanol, dry	4.880	na		na
	EtOAc dry	0.203	-0.335	1.251	2.949	0.000	0.917	0.000	L	EtOAc/Dry/Oct 99	4.247	na		na
MECN-1	MeCN, dry	-0.007	-0.595	2.461	2.085	0.418	0.738	0.000	L	MeCN/dry/June 99	4.397	na		na
	NFM-B	-0.624	0.016	2.477	3.989	0.000	0.692	0.000	L	NFM-B	3.677	na		na
MHA	DMF, dry	-0.161	-0.189	2.327	4.756	0.000	0.808	0.000	L	DMF/Dry/Sept 98	4.360	na		na
	Acetone dry	0.154	-0.277	1.522	3.258	0.078	0.863	0.000	L	Acetone/Dry/August 99	4.266	na		na
	IOA	-0.548	-0.227	0.107	0.164	0.000	0.198	0.000	L	IOA	0.145	na		na
	NMP	-0.293	0.253	2.210	5.094	0.000	0.818	0.000	L	NMP/dry/Sept 98	4.340	na		na
	Nitromethane, dry	-0.340	-0.297	2.689	2.193	0.514	0.728	0.000	L	Nitromethane, dry	4.352	na		na
	DMSO, dry	-0.619	0.131	2.811	5.474	0.000	0.734	0.000	L	DMSO, dry	4.123	na		na
	OV1	0.705	0.000	0.746	0.683	0.000	2.001	0.000	I/100	OV1/10 Quest	8.312	na		na
	PEG	-5.496	0.960	5.629	8.841	0.000	2.037	0.000	I/100	PEG/10 Quest	6.259	na		na
	SE54	0.578	-0.419	1.430	0.983	0.000	2.010	0.000	I/100	SE54/10 Quest	8.576	na		na
	TEG	-2.731	0.208	1.882	4.632	0.313	0.584	0.000	L	TEG Rachel Old Best	0.950	na		na
	DBS	-2.034	0.000	0.968	1.911	0.045	0.765	0.000	L	DBS Rachel New Best	1.406	na		na
	BDS Squalane	0.815	-0.580	0.950	0.000	0.000	1.952	0.000	I/100	BDS, Squalane	8.187	na		na
	WangA	0.718	-0.180	0.854	0.768	0.000	1.983	0.000	I/100	WangA	8.275	na		na
	WangB	0.715	-0.179	0.835	0.417	0.000	1.982	0.000	I/100	WangB	8.256	na		na
	Wang2A	0.560	0.980	5.686	9.450	0.000	2.001	0.000	I/100	Wang2	12.237	na		na
	Water,37	-1.361	1.055	2.630	3.742	4.495	-0.245	0.000	logL	Water,37	2.074	na		na
	Blood,37	-1.269	0.612	0.916	3.614	3.381	0.362	0.000	logL	Blood,37	2.375	na		na
	Liver,37	-1.031	0.059	0.774	0.593	1.049	0.654	0.000	logL	Liver,37	2.326	na		na
	Muscle,37	-1.140	0.544	0.216	3.471	2.924	0.578	0.000	logL	Muscle,37	2.518	na		na
	Fat,37	-0.294	-0.172	0.729	1.747	0.219	0.895	0.000	logL	Fat,37	3.435	na		na
JAFC (1989) 37(3)	SE-54	0.711	-0.377	1.042	1.019	0.219	1.985	0.000	RI/100	SE-54	8.438	8.438	8.490	0.003
JAFC (1990) 38(2)	DB-1	0.380	-0.578	0.926	0.631	0.890	1.994	0.000	RI/100	DB-1	8.266	8.266	8.310	0.002
JAFC (1991) 39(7)	DB-5	0.674	0.000	1.555	0.957	0.000	1.991	0.000	RI/100	DB-5	8.853	na		na
JAFC (1991) 39(11) 1972-1975		0.465	-1.373	4.806	1.418	-4.049	2.009	0.000	RI/100		8.894	na		na
JAFC (2001) 49(3) 1345-1352		-0.544	-0.522	1.503	1.294	0.000	2.010	0.000	RI/100		7.469	na		na
JAFC (2001) 49(12	AT-WAX	-0.549	0.959	6.556	10.322	-0.839	2.171	0.000	RI/100		12.011	12.011	12.060	0.002
JAFC (2001) 49(12	CP-SIL-5CB	0.491	-0.511	1.164	1.206	-0.377	2.056	0.000	RI/100		8.254	8.254	8.170	0.007
JAFC (2001) 49(12	AT-WAX	-0.603	0.721	6.999	10.571	-1.285	2.169	0.000	RI/100	AT-WAX	12.002	12.002	12.060	0.003
JAFC (2001) 49(12	CP-SIL-5CB	0.367	-0.590	1.188	1.143	-0.319	2.084	0.000	RI/100	CP-SIL-5CB	8.242	8.242	8.170	0.005
JAFC (2003) 51(5)	DB-5	0.707	0.000	1.225	1.325	0.000	1.972	0.000	RI/100	DB-5	8.572	8.572	8.560	0.000
Food Chem (2004)	CP-SIL-8CB	0.532	-0.473	1.552	1.340	-0.344	2.030	0.000	RI/100	CP-SIL-8CB	8.522	8.522	8.480	0.002
Flav Frag J (2003)	DB-5	0.850	0.000	0.951	1.143	0.000	1.970	0.000	RI/100	DB-5	8.502	8.502	8.540	0.001
JAFC (2003) 51(7)	DB-Wax	0.657	0.000	6.952	10.389	-1.377	1.979	0.000	RI/100	DB-Wax	12.250	12.250	12.210	0.002
	PENGA	0.053	-0.045	0.145	0.065	-0.007	0.201	0.000	trel	PENGA	0.850	na		na
	PENGB	0.034	0.021	0.283	0.088	0.028	0.203	0.000	I/1000	PENGB	0.981	na		na
	PENGC	0.044	0.046	0.303	0.118	0.050	0.202	0.000	I/1001	PENGC	1.021	na		na

PENGD	0.035	0.050	0.316	0.104	0.041	0.203	0.000	I/1002	PENGD	1.023	na	na
PENGE	0.037	-0.115	0.524	0.130	0.063	0.203	0.000	I/1003	PENGE	1.129	na	na
PENGF	0.012	0.011	0.582	0.503	-0.011	0.206	0.000	I/1004	PENGF	1.173	na	na
PENGG	0.025	-0.040	0.782	1.116	-0.185	0.204	0.000	I/1005	PENGG	1.236	na	na
PENGH	0.022	0.041	0.693	0.931	-0.067	0.204	0.000	I/1006	PENGH	1.247	na	na
WSA-1	0.061	-0.076	0.847	1.116	-0.035	0.199	0.000	I/1007	WSA-1	1.354	na	na
FFAP	0.050	0.136	0.575	1.024	0.000	0.200	0.000	I/1008	FFAP	1.236	na	na
SE34	0.078	-0.008	0.116	0.185	0.000	0.197	0.000	I/1009	SE34	0.856	na	na
MLT	0.087	0.055	0.076	0.126	0.000	0.197	0.000	I/1000	MLT	0.857	na	na
JEA	0.053	-0.027	0.122	0.093	0.000	0.203	0.000	I/1000	JEA	0.850	na	na
GLCH-6	0.933	2.087	5.269	6.766	0.000	1.835	0.000	I/100	GLCH-6	12.125	na	na
B245	0.073	0.014	0.428	0.480	0.000	0.198	0.000	I/100	B245 June 98	1.095	na	na
B267	0.208	0.001	0.750	0.741	0.000	0.166	0.000	I/100	B267 June 98	1.354	na	na
B196	0.105	0.014	0.169	0.255	0.000	0.189	0.000	I/100	B196-1	0.901	na	na
HP	0.060	-0.044	0.281	0.303	0.000	0.197	0.000	I/1000	HP	0.950	na	na
TAKA	0.483	1.070	5.669	8.801	0.000	2.009	0.000	I/100	TAKA June 98	12.208	na	na
GTA	0.595	-0.137	0.881	1.102	0.000	2.006	0.000	I/100	GTA June 98	8.271	na	na
GTB	0.573	-0.089	0.833	0.931	0.000	2.009	0.000	I/100	GTB June 98	8.241	na	na
SCHA	0.487	-0.544	0.941	1.470	0.000	2.077	0.000	I/100	SCHA June 98	8.305	na	na
SCHB	0.413	-0.552	1.022	1.533	0.000	2.105	0.000	I/100	SCHB June 98	8.388	na	na
CARBO	-1.983	0.259	1.254	2.022	0.000	0.423	0.000	I-rel	CARBO June 98	0.544	na	na
DEGS	-1.797	0.348	1.597	1.874	0.000	0.388	0.000	I-rel	DEGS June 98	0.897	na	na
POLY	-2.472	0.133	0.884	0.597	0.000	0.539	0.000	I-rel	POLY June 98	0.139	na	na
TCEP	-1.664	0.242	1.939	1.894	0.000	0.366	0.000	I-rel	TCEP June 98	1.169	na	na
Zonyl	-1.979	-0.441	1.471	0.771	0.000	0.431	0.000	I-rel	Zonyl June 98	0.478	na	na
JB2A	0.739	0.000	0.243	0.000	0.000	1.977	0.000	I/100	JB2A	7.886	na	na
JB2F	0.696	-0.401	3.160	0.000	0.000	1.986	0.000	!/100	JB2F	9.911	na	na
JBA	0.727	0.000	0.000	0.000	0.000	1.980	0.000	I/100	JBA	7.702	na	na
JBF	0.716	-0.612	3.216	0.000	0.000	1.981	0.000	I/100	JBF	9.878	na	na
GCD	0.249	0.654	6.820	8.962	0.000	2.044	0.000	I/100	GCD August 98	12.805	na	na
RTXCI	-0.092	0.912	6.543	9.465	0.000	2.061	0.000	I/100	RTXCI	12.412	na	na
RTXBI	0.251	-1.727	4.431	0.910	0.000	2.095	0.000	I/100	RTXBI	10.311	na	na
RTXAI	0.431	-0.164	1.056	0.723	0.000	2.037	0.000	I/100	RTXAI	8.337	na	na
FPOL 298	-1.207	-0.672	1.446	1.494	4.086	0.810	0.000	logK	FPOL 298	4.238	na	na
FPOL 333	-0.527	-0.464	1.152	0.908	2.645	0.611	0.000	logK	FPOL 333	3.454	na	na
18-1	-0.510	-0.070	1.360	1.210	0.830	0.931	0.000	logL	18-1	4.120	na	na
18-2	0.260	-0.010	0.990	1.390	0.700	0.967	0.000	logL	18-2	4.706	na	na
18-6	-0.340	-0.460	1.220	1.060	1.160	0.882	0.000	logL	18-6	4.009	na	na
18-7	-0.160	-0.230	1.010	1.040	1.140	0.956	0.000	logL	18-7	4.369	na	na
18-9	-1.210	-0.380	1.380	0.710	5.310	0.984	0.000	logL	18-9	5.433	na	na
18-11	-0.180	0.000	1.180	1.500	1.330	0.931	0.000	logL	18-11	4.556	na	na
18-12	0.390	0.080	1.010	0.820	0.360	0.923	0.000	logL	18-12	4.583	na	na
18-13	-0.750	0.070	1.140	1.280	1.890	0.934	0.000	logL	18-13	4.234	na	na
18-14	-0.060	-0.560	0.910	1.400	2.760	0.846	0.000	logL	18-14	4.581	na	na
18-15	-1.080	-0.200	0.870	1.800	3.420	0.899	0.000	logL	18-15	4.135	na	na
cooka	0.639	1.459	0.000	0.000	0.000	1.995	0.000	I/100	cooka	8.208	na	na

cookb	0.658	1.126	0.144	0.000	0.000	1.991	0.000	I/100	cookb	8.196	na	na
cookc	0.589	0.156	1.026	0.000	0.000	2.008	0.000	I/100	cookc	8.490	na	na
cookd	0.653	0.091	0.867	0.897	0.000	1.995	0.000	I/100	cookd	8.366	na	na
cooke	0.658	0.595	0.000	0.000	0.000	1.993	0.000	I/100	cooke	7.900	na	na
NNVA	0.853	0.884	0.000	0.000	0.000	1.958	0.000	I/100	NNVA	8.078	na	na
NNVB	0.797	0.756	2.069	0.000	0.000	1.967	0.000	I/100	NNVB	9.559	na	na
NNVC	0.991	0.729	5.428	0.000	0.000	1.934	0.000	I/100	NNVC	12.146	na	na
K78	0.665	0.859	0.000	0.000	0.000	1.998	0.000	I/100	K78	8.022	na	na
KOH	0.641	0.884	0.322	0.497	0.565	2.002	0.000	I/100	KOH	8.506	na	na
Kidney	-1.084	0.417	0.226	3.624	2.926	0.534	0.000	logL	Kidney 37	2.380	na	na
Brain	-1.074	0.427	0.286	2.781	2.787	0.609	0.000	logL	Brain 37	2.643	na	na
ODT	0.000	0.564	1.682	1.583	1.522	0.751	0.000	log1/ODT	ODT c=0	4.771	na	na

a M.H.Abraham, J.Phys.Org.Chem., 1994, 6, 660-684.
b M.H.Abraham, H.S.Chadha, J.Dixon and A.J.Leo, J.Phys.Org.Chem., 1994, 7, 712.
c M.H.Abraham, unpublished equation.
d M.H.Abraham, J.Andonian-Haftvan, G.S.Whiting, A.Leo and R.W.Taft, J.Chem.Soc.Perkin Trans 2, 1994, 1777.
e M.H.Abraham, H.S.Chadha and R.C.Mitchell, J.Pharm.Sci., 1994, 83,
f J.A.Gratton, M.H.Abraham, M.W.Bradbury and H.S.Chadha, submitted.
g M.H.Abraham, F.Martins and R.C.Mitchell, J.Pharm.Pharmacol., 1997,
h A.Pagliara, G.Caron, G.Lisa, W.Fan, P.Gaillard, P.-A.Carrupt, B.Testa and M.H.Abraham, J.Chem.Soc., Faraday Trans., submitted.
i M.H.Abraham, K.Takacs-Novak and R.C.Mitchell, J.Pharm.Sci., 1997, 86,