Supplementary Material

Gas principal properties as new compact descriptors for data-driven gas solubility modelling

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Table S1 Statistical parameters for the PCA model adopted to derive gas PPs (48 objects, 42 variables).

PC	R2X	R2X(cum)	Q2	Q2(cum)
1	0.440	0.440	0.243	0.243
2	0.248	0.688	0.324	0.488
3	0.149	0.837	0.335	0.660
4	0.060	0.897	0.175	0.719

Table S2 Numerical values of descriptors and of the dependent variable in Henry solubility PLS model.

entry	gas/solvent	Set	PP1, solv	PP1, gas	PP2, gas	PP3, gas	logH	*pred* logH
CH4/PhNH2	methane/aniline	L	0.39	-2.45	0.96	1.99	3.20	2.93
CH4/PhCH2OH	methane/benzyl alcohol	L	0.71	-2.45	0.96	1.99	3.01	2.97
CH4/DMSO	methane/dimethylsulfoxide	L	3.19	-2.45	0.96	1.99	3.39	3.31
CH4/Et(OH)2	methane/ethylene glycol	L	3.06	-2.45	0.96	1.99	3.76	3.29
CH4/HMPT	methane/hexamethyl phosphoramide	L	2.76	-2.45	0.96	1.99	2.67	3.25
CH4/PhNO2	methane/nitrobenzene	L	0.92	-2.45	0.96	1.99	2.97	3.00
C2H4/PhNH2	ethylene/aniline	L	0.39	-1.40	0.53	2.54	2.32	2.07
C2H4/Dec.	ethylene/decalin	L	-3.64	-1.40	0.53	2.54	1.86	1.52
C2H4/DMSO	ethylene/dimethylsulfoxide	L	3.19	-1.40	0.53	2.54	2.49	2.45
C2H4/Et(OH)2	ethylene/ethylene glycol	L	3.06	-1.40	0.53	2.54	2.88	2.43
C2H4/HMPT	ethylene/hexamethylphosphoramide	L	2.76	-1.40	0.53	2.54	1.72	2.39
C2H4/NMePyrr	ethylene/1-methyl-2-pyrrolidone	L	2.17	-1.40	0.53	2.54	2.10	2.31
C2H4/PhNO2	ethylene/nitrobenzene	L	0.92	-1.40	0.53	2.54	2.10	2.14
Pr/PhNH2	propane/nitrobenzene	L	0.39	1.02	2.68	0.43	1.85	1.70
Pr/PhCH2OH	propane/benzyl alcohol	L	0.71	1.02	2.68	0.43	1.71	1.74
Pr/Dec.	propane/decalin	L	-3.64	1.02	2.68	0.43	1.08	1.15
Pr/DMSO	propane/dimethylsulfoxide	L	3.19	1.02	2.68	0.43	2.27	2.08
Pr/HMPT	propane/hexamethyl phosphoramide	L	2.76	1.02	2.68	0.43	1.30	2.02
Pr/NMePyrr	propane/1-methyl-2-pyrrolidone	L	2.17	1.02	2.68	0.43	1.76	1.94
Pr/PhNO2	propane/nitrobenzene	L	0.92	1.02	2.68	0.43	1.64	1.77
nBu/PhNH2	n-butane/aniline	L	0.39	2.42	3.55	-0.17	1.40	1.21
nBu/PhCH2OH	n-butane/benzyl alchol	L	0.71	2.42	3.55	-0.17	1.20	1.26
nBu/Dec.	n-butane/decalin	L	-3.64	2.42	3.55	-0.17	0.55	0.66
nBu/DMSO	n-butane/dimethylsulfoxide	L	3.19	2.42	3.55	-0.17	1.81	1.59

nBu/Et(OH)2	n-butane/ethylen glycol	L	3.06	2.42	3.55	-0.17	2.43	1.58
nBu/NMePyrr	n-butane/1-methyl-2-pyrrolidone	L	2.17	2.42	3.55	-0.17	1.26	1.45
nBu/PhNO2	n-butane/nitrobenzene	L	0.92	2.42	3.55	-0.17	1.13	1.28
Et/PhNH2	ethane/aniline	L	0.39	-0.95	1.35	1.95	2.26	2.12
Et/PhCH2OH	ethane/benzyl alcohol	L	0.71	-0.95	1.35	1.95	2.16	2.16
Et/Dec.	ethane/decaline	L	-3.64	-0.95	1.35	1.95	1.65	1.57
Et/DMSO	ethane/dimethylsulfoxide	L	3.19	-0.95	1.35	1.95	2.59	2.50
Et/Et(OH)2	ethane/ethylene glycol	L	3.06	-0.95	1.35	1.95	2.79	2.48
Et/NMePyrr	ethane/1-methyl-2-methylpyrrolidone	L	2.17	-0.95	1.35	1.95	2.17	2.36
Et/PhNO2	ethane/nitrobenzene	L	0.92	-0.95	1.35	1.95	2.11	2.19
iBu/PhCH2OH	isobutane/benzyl alcohol	L	0.71	2.30	3.26	-0.43	1.49	1.39
iBu/Dec.	isobutane/decalin	L	-3.64	2.30	3.26	-0.43	0.73	0.80
iBu/DMSO	isobutane/dimethylsulfoxide	L	3.19	2.30	3.26	-0.43	2.15	1.73
iBu/Et(OH)2	isobutane/ethylene glycol	L	3.06	2.30	3.26	-0.43	2.51	1.71
iBu/HMPT	isobutane/hexamethyl phosphoramide	L	2.76	2.30	3.26	-0.43	1.02	1.67
iBu/NMePyrr	isobutane/1-methyl-2-pyrrolidone	L	2.17	2.30	3.26	-0.43	1.52	1.59
iBu/PhNO2	isobutane/nitrobenzene	L	0.92	2.30	3.26	-0.43	1.39	1.42
C3H6/PhNH2	propene/aniline	L	0.39	0.74	2.39	0.78	1.64	1.70
C3H6/PhCH2OH	propene/benzyl alcohol	L	0.71	0.74	2.39	0.78	1.57	1.74
C3H6/Dec.	propene/decaline	L	-3.64	0.74	2.39	0.78	1.15	1.15
C3H6/DMSO	propene/dimethylsulfoxide	L	3.19	0.74	2.39	0.78	1.97	2.08
C3H6/Et(OH)2	propene/ethylene glycol	L	3.06	0.74	2.39	0.78	2.31	2.06
C3H6/HMPT	propene/hexamethyl phosphoramide	L	2.76	0.74	2.39	0.78	1.13	2.02
C3H6/PhNO2	propene/nitrobenzene	L	0.92	0.74	2.39	0.78	1.49	1.77
CH4/Dec.	methane/decaline	T	-3.64	-2.45	0.96	1.99	2.54	2.38
CH4/NMePyrr	methane/1-methyl-2-pyrrolidone	T	2.17	-2.45	0.96	1.99	3.01	3.17
C2H4/PhCH2OH	ethylene/benzyl alcohol	T	0.71	-1.40	0.53	2.54	2.20	2.11
Pr/Et(OH)2	propane/ethylene glycol	T	3.06	1.02	2.68	0.43	2.61	2.06
nBu/HMPT	n-butane/hexamethyl phosphoramide	T	2.76	2.42	3.55	-0.17	0.78	1.54
Et/HMPT	ethane/hexamethyl phosphoramide	T	2.76	-0.95	1.35	1.95	1.76	2.44
iBu/PhNH2	isobutane/aniline	T	0.39	2.30	3.26	-0.43	1.64	1.35
C3H6/NMePyrr	propene/1-methyl-2-pyrrolidone	T	2.17	0.74	2.39	0.78	1.49	1.94
CO2/PhNH2	carbon dioxide/aniline	E	0.39	-0.16	-1.68	3.97	2.10	
CO2/PhCH2OH	carbon dioxide/benzyl alcohol	E	0.71	-0.16	-1.68	3.97	2.11	
CO2/Dec.	carbon dioxide/decalin	E	-3.64	-0.16	-1.68	3.97	2.04	
CO2/DMSO	carbon dioxide/dimethylsulfioxide	E	3.19	-0.16	-1.68	3.97	2.03	
CO2/Et(OH)2	carbon dioxide/ethylene glycol	E	3.06	-0.16	-1.68	3.97	2.42	
CO2/HMPT	carbon dioxide/hexamethyl phosphoramide	E	2.76	-0.16	-1.68	3.97	1.48	
CO2/NMePyrr	carbon dioxide/1-methyl-2-pyrrolidone	E	2.17	-0.16	-1.68	3.97	1.77	
CO2/PhNO2	carbon dioxide/nitrobenzene	E	0.92	-0.16	-1.68	3.97	1.88	
H2S/PhNH2	hydrogen sulfide/aniline	E	0.39	0.18	0.29	2.95	1.18	
H2S/PhCH2OH	hydrogen sulfide/benzyl alchol	E	0.71	0.18	0.29	2.95	1.38	
H2S/Dec.	hydrogen sulfide/decaline	E	-3.64	0.18	0.29	2.95	1.47	
H2S/DMSO	hydrogen sulfide/dimethylsulfoxide	E	3.19	0.18	0.29	2.95	1.04	
H2S/Et(OH)2	hydrogen sulfide/ethylene glycol	E	3.06	0.18	0.29	2.95	1.72	
H2S/HMPT	hydrogen sulfide/hexamethyl phosphoramide	E	2.76	0.18	0.29	2.95	0.21	
H2S/NMePyrr	hydrogen sulfide/1-methyl-2-pyrrolidone	E	2.17	0.18	0.29	2.95	0.75	
H2S/PhNO2	hydrogen sulfide/nitrobenzene	E	0.92	0.18	0.29	2.95	1.27	
SO2/PhCH2OH	sulfur dioxide/benzyl alcohol	E	0.71	2.42	0.35	1.41	0.32	
SO2/Dec.	sulfur dioxide/decalin	E	-3.64	2.42	0.35	1.41	1.27	
SO2/DMSO	sulfur dioxide/dimethylsulfoxide	E	3.19	2.42	0.35	1.41	-0.93	
SO2/Et(OH)2	sulfur dioxide/ethylene glycol	E	3.06	2.42	0.35	1.41	0.53	
SO2/PhNO2	sulfur dioxide/nitrobenzene	E	0.92	2.42	0.35	1.41	0.21	

L= learning set; T= test set; E= excluded from the hydrocarbons model

Figure S1 Scores plot for the Henry solubility model including all gases

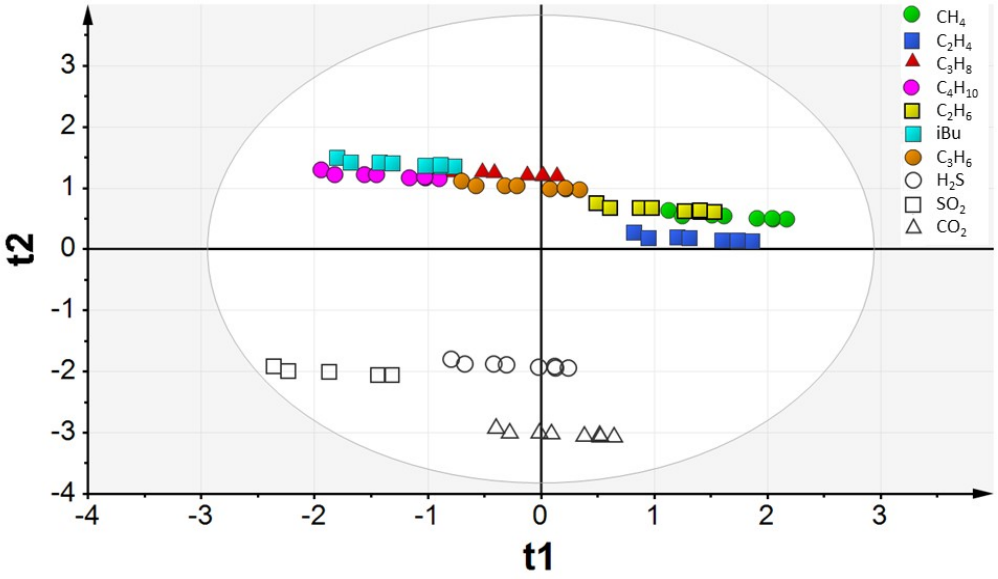

Table S3 PLS statistical parameters for the 6 descriptors Henry solubility model.

PC	R2X	R2X(cum)	R2Y	R2Y(cum)	Q2	Q2(cum)
1	0.485	0.485	0.575	0.575	0.547	0.547
2	0.252	0.737	0.075	0.650	0.118	0.601

Figure S2 VIP bar plot for the 6 descriptors Henry solubility PLS model.

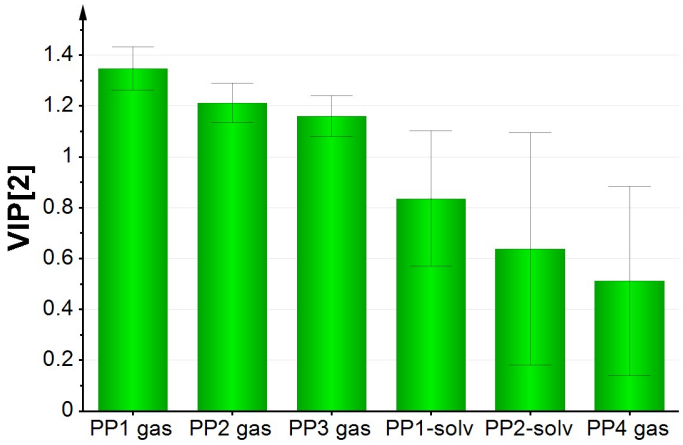

Table S4 PLS statistical parameters for the 4 descriptors Henry solubility model.

PC	R2X	R2X(cum)	R2Y	R2Y(cum)	Q2	Q2(cum)
1	0.715	0.715	0.58	0.58	0.547	0.547
2	0.267	0.982	0.0857	0.666	0.182	0.63
3	0.0146	0.997	0.102	0.768	0.271	0.73

Figure S3 VIP bar plot for the 4 descriptors Henry solubility PLS model

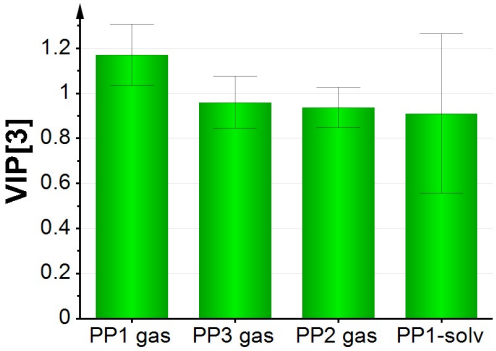

Table S5 Numerical values of descriptors and of the dependent variable in the Ostwald solubility PLS model.

gas/alchol	Set	PP1, solv	PP2, solv	PP1, gas	PP2, gas	PP3, gas	PP4, gas	Log*L*	pred. Log*L*
Ar/EtOH	L	1.11	-2.71	-2.52	-5.59	1.22	-0.93	-0.58	-0.70
Ar/nBuOH	L	0.52	-1.47	-2.52	-5.59	1.22	-0.93	-0.62	-0.70
Ar/nPentOH	L	0.15	-0.92	-2.52	-5.59	1.22	-0.93	-0.64	-0.70
Ar/nPrOH	L	0.78	-2.35	-2.52	-5.59	1.22	-0.93	-0.61	-0.70
CH4/EtOH	L	1.11	-2.71	-2.45	0.96	1.99	-1.68	-0.29	-0.35
CH4/nBuOH	L	0.52	-1.47	-2.45	0.96	1.99	-1.68	-0.31	-0.35
CH4/nPentOH	L	0.15	-0.92	-2.45	0.96	1.99	-1.68	-0.33	-0.35
CH4/nPrOH	L	0.78	-2.35	-2.45	0.96	1.99	-1.68	-0.29	-0.35
He/EtOH	L	1.11	-2.71	-10.38	-1.97	-5.09	-1.16	-1.52	-1.55
He/MetOH	L	1.63	-3.04	-10.38	-1.97	-5.09	-1.16	-1.46	-1.55
He/nPentOH	L	0.15	-0.92	-10.38	-1.97	-5.09	-1.16	-1.63	-1.55
He/nPrOH	L	0.78	-2.35	-10.38	-1.97	-5.09	-1.16	-1.56	-1.55
Kr/EtOH	L	1.11	-2.71	-0.45	-6.87	-0.14	1.15	-0.16	-0.05
Kr/MeOH	L	1.63	-3.04	-0.45	-6.87	-0.14	1.15	-0.19	-0.05
Kr/nPentOH	L	0.15	-0.92	-0.45	-6.87	-0.14	1.15	-0.19	-0.05
Kr/nPrOH	L	0.78	-2.35	-0.45	-6.87	-0.14	1.15	-0.16	-0.05
N2/EtOH	L	1.11	-2.71	-2.53	-2.34	1.12	-2.27	-0.84	-0.75
N2/MeOH	L	1.63	-3.04	-2.53	-2.34	1.12	-2.27	-0.81	-0.75
N2/nBuOH	L	0.52	-1.47	-2.53	-2.34	1.12	-2.27	-0.91	-0.75
N2/nPrOH	L	0.78	-2.35	-2.53	-2.34	1.12	-2.27	-0.88	-0.75

Ne/EtOH	L	1.11	-2.71	-6.23	-7.84	1.75	-1.07	-1.36	-1.42
Ne/MeOH	L	1.63	-3.04	-6.23	-7.84	1.75	-1.07	-1.32	-1.42
Ne/nBuOH	L	0.52	-1.47	-6.23	-7.84	1.75	-1.07	-1.45	-1.42
Ne/nPentOH	L	0.15	-0.92	-6.23	-7.84	1.75	-1.07	-1.49	-1.42
Ne/nPrOH	L	0.78	-2.35	-6.23	-7.84	1.75	-1.07	-1.42	-1.42
O2/nBuOH	L	0.52	-1.47	-2.56	-3.40	1.49	-1.58	-0.67	-0.68
O2/nPentOH	L	0.15	-0.92	-2.56	-3.40	1.49	-1.58	-0.70	-0.68
O2/nPrOH	L	0.78	-2.35	-2.56	-3.40	1.49	-1.58	-0.66	-0.68
Xe/nBuOH	L	0.52	-1.47	0.53	-7.44	-1.16	2.00	0.41	0.23
Xe/nPentOH	L	0.15	-0.92	0.53	-7.44	-1.16	2.00	0.39	0.23
CH4/MeOH	T	1.63	-3.04	-2.45	0.96	1.99	-1.68	-0.30	-0.35
He/nBuOH	T	0.52	-1.47	-10.38	-1.97	-5.09	-1.16	-1.59	-1.55
Kr/nBuOH	T	0.52	-1.47	-0.45	-6.87	-0.14	1.15	-0.17	-0.05
N2/nPentOH	T	0.15	-0.92	-2.53	-2.34	1.12	-2.27	-0.94	-0.75
O2/EtOH	T	1.11	-2.71	-2.56	-3.40	1.49	-1.58	-0.62	-0.68
Xe/nPrOH	T	0.78	-2.35	0.53	-7.44	-1.16	2.00	0.38	0.23
SF6/MeOH	E	1.63	-3.04	3.55	-0.89	-2.73	1.76	-0.21	
SF6/EtOH	E	1.11	-2.71	3.55	-0.89	-2.73	1.76	-0.12	
SF6/nPrOH	E	0.78	-2.35	3.55	-0.89	-2.73	1.76	-0.13	
SF6/nBuOH	E	0.52	-1.47	3.55	-0.89	-2.73	1.76	-0.17	
SF6/nPentOH	E	0.15	-0.92	3.55	-0.89	-2.73	1.76	-0.21	

L= learning set; T= test set; E= experiments with SF_6 excluded from the Ostwald solubility model

Table S6 PLS statistical parameters for the Ostwald solubility model.

PC	R2X	R2X(cum)	R2Y	R2Y(cum)	Q2	Q2(cum)
1	0.323	0.323	0.757	0.757	0.670	0.670
2	0.187	0.510	0.191	0.949	0.752	0.918
3	0.221	0.730	0.025	0.974	0.362	0.948