

Experimental and calculated using the CORAL values of solubility, S, [mg/mL].

No.	SMILES	DCW(1)	S <sub>Expr</sub>	S <sub>Calc</sub>	S <sub>Expr</sub> -S <sub>Calc</sub>
	<b>Training set</b>				
1	O=C(OC)CCCC%21(c1cccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	225.5672352	50.000	23.128	26.872
2	O=C(OCC)CCCC%21(c1cccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	226.7408106	19.000	31.498	-12.498
4	O=C(OC)CCCC%31(c1cccc1)C%28%30C%26C=%20C=%32C=%19C%33=C%10c3c9c2c8c7c6c5c2c4c3C%33=C%18C=%17C4=C5C%16=C%15C6=C%14C7=C%13C=%12C8=C9C%11=C%10C=%32C%27=C%11C=%12C%25=C%13C%24=C%14C%23=C%15C%22=C%16C=%17C%21=C%18C=%19C=%20C%29C%21=C%22C(=C%23C%24=C%28C%25=C%26%27)C%29%30%31	230.4714368	58.000	58.107	-0.107
5*	O=C(OC)CCCC%37(c1cccc1)C%32%38C4c%36c3c2c%34C%21=C%18c2c%14c%16c3C4=C%31C%17C%10=C%30C=%29C=9c8c%22c%24c7e5c%25c%27c%20c6c%19c%13c%12c(c56)c7c8C=%11C=9C%10=C%15C(C=%11%12)=C%13C(C%14=C%15C%16%17)=C%18C%19=C%20C%21=C%28C%35=C%33C%26=C%23C(=C(C=%29C%22=C%23c%24c%25C%26=C%27%28)C%32=C%30%31)C%37%38C%33c%36c%34%35	226.7805714	80.000	31.782	48.218
7	O=C(OCC)CCC%21(c1cccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	225.5672352	5.000	23.128	-18.128
8	O=C(OCCC)CCC%21(c1cccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	226.7408106	43.000	31.498	11.502
10	O=C(OCCCC)CCC%21(c1cccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	227.9143860	30.000	39.869	-9.869
11	O=C(OCe1cccc1)CCC%22(c2cccc2)C%33%23C%32C=%20C=%34C=%18C%16=C6c5c%15c%14c%13c4c3c%12C%11=C9C=8C3=C(c45)C7=C6C=%34C%31=C7C=8C%30=C9C=%29C(C%10=C%21C=%17C=%25C%28=C%10C=%29C%11=C%27c%12c%13C%26=C%14C=%24C(=C%15%16)C%19=C(C=%17C(C=%20C=%18%19)C%21%22%23)C=%24C=%25C%26=C%27%28)=C%33C%30=C%31%32	237.3108178	106.000	106.888	-0.888
13	O=C(OC)CCC%37(c1cccc1)C%32%38C4c%36c3c2c%34C%21=C%18c2c%14c%16c3C4=C%31C%17C%10=C%30C=%29C=9c8c%22c%24c7e5c%25c%27c%20c6c%19c%13c%12c(c56)c7c8C=%11C=9C%10=C%15C(C=%11%12)=C%13C(C%14=C%15C%16%17)=C%18C%19=C%20C%21=C%28C%35=C%33C%26=C%23C(=C(C=%29C%22=C%23c%24c%25C%26=C%27%28)C%32=C%30%31)C%37%38C%33c%36c%34%35	225.6069960	12.000	23.411	-11.411
14	O=C(OCC)CCC%37(c1cccc1)C%32%38C4c%36c3c2c%34C%21=C%18c2c%14c%16c3C4=C%31C%17C%10=C%30C=%29C=9c8c%22c%24c7e5c%25c%27c%20c6c%19c%13c%12c(c56)c7c8C=%11C=9C%10=C%15C(C=%11%12)=C%13C(C%14=C%15C%16%17)=C%18C%19=C%20C%21=C%28C%35=C%33C%26=C%23C(=C(C=%29C%22=C%23c%24c%25C%26=C%27%28)C%32=C%30%31)C%37%38C%33c%36c%34%35	226.7805714	10.000	31.782	-21.782
16	O=C(OCCCC)CCC%37(c1cccc1)C%32%38C4c%36c3c2c%34C%21=C%18c2c%14c%16c3C4=C%31C%17C%10=C%30C=%29C=9c8c%22c%24c7e5c%25c%27c%20c6c%19c%13c%12c(c56)c7c8C=%11C=9C%10=C%15C(C=%11%12)=C%13C(C%14=C%15C%16%17)=C%18C%19=C%20C%21=C%28C%35=C%33C%26=C%23C(=C(C=%29C%22=C%23c%24c%25C%26=C%27%28)C%32=C%30%31)C%37%38C%33c%36c%34%35	229.1277222	30.000	48.523	-18.523

17	O=C(OCC)CCC%31(c1cccs1)C%28%30C%26C=%20C=%32C=%19C%33=C%10c3c9c2e8c7c6c5e2c4c3C%33=C%18C=%17C4=C5C%16=C%15C6=C%14C7=C%13C=%12C8=C9C%11=C%10C=%32C%27=C%11C=%12C%25=C%13C%24=C%14C%23=C%15C%22=C%16C=%17C%21=C%18C=%19C=%20C%29C%21=C%22C(=C%23C%24=C%28C%25=C%26%27)C%29%30%31	228.0257611	23.000	40.663	-17.663
19	O=C(OCCCC)CCC%31(c1cccs1)C%28%30C%26C=%20C=%32C=%19C%33=C%10c3c9c2e8c7c6c5e2c4c3C%33=C%18C=%17C4=C5C%16=C%15C6=C%14C7=C%13C=%12C8=C9C%11=C%10C=%32C%27=C%11C=%12C%25=C%13C%24=C%14C%23=C%15C%22=C%16C=%17C%21=C%18C=%19C=%20C%29C%21=C%22C(=C%23C%24=C%28C%25=C%26%27)C%29%30%31	230.3729119	70.000	57.404	12.596
20	O=C(OCCC)CCC%38(c1cccs1)C%36%37C%28c%11c%27e2c%26C%23=C%34c2c%12C=%10C=%35C=9c%21c8c3c%20c%19c4c3c7c6c5c4C=%18C%17=C5C%16=C%15C6=C%13c7c8C=9C=%14C=%10C(=C%11%12)C%37%38C(C%13=%14)=C%15C%36=C%29C%16=C%30C%17=C%33C=%25C=%18c%19c%24c%22c%20c%21C(=C%22C%23=C(C%24=%25)C=%32c%26c%31c%27C%28=C%29C%30C%31C=%32%33)C%34=%35	239.9065824	130.000	125.402	4.598
22	CCCCCCC%21(c1ccccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	226.9315069	31.000	32.858	-1.858
23	CCCCC%21(c1ccccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	224.5843561	23.000	16.118	6.882
25	[O-]C(=O)CCC%26(CCC([O-])=O)C%32%25C%15=C%13C=%21C%12=C%23C=3C=%11c2c%10c9c1e8c7c6c4c1c2C=5C=3C=%22C%18=C(C4=5)C%17=C6C%16=C7C%27=C%29C8=C9C=%30C%14=C%10C=%11C%12=C%13C%14=C%31C%15=C%28C%32C=%20C(C%16=C%19C%17=C%18C=%24C(C%19=%20)C%25%26C=%21C=%24C=%22%23)=C%27C%28=C%29C=%30%31	222.8770135	4.000	3.940	0.060
26	O=C(OCC)C%26(C(=O)OCCOC)C%32%25C%15=C%13C=%21C%12=C%23C=3C=%11c2c%10c9c1e8c7c6c4c1c2C=5C=3C=%22C%18=C(C4=5)C%17=C6C%16=C7C%27=C%29C8=C9C=%30C%14=C%10C=%11C%12=C%13C%14=C%31C%15=C%28C%32C=%20C(C%16=C%19C%17=C%18C=%24C(C%19=%20)C%25%26C=%21C=%24C=%22%23)=C%27C%28=C%29C=%30%31	223.5862542	11.000	8.999	2.001
	<b>Validation set</b>				
3	O=C(O)CCCC%31(c1cccs1)C%28%30C%26C=%20C=%32C=%19C%33=C%10c3c9c2e8c7c6c5e2c4c3C%33=C%18C=%17C4=C5C%16=C%15C6=C%14C7=C%13C=%12C8=C9C%11=C%10C=%32C%27=C%11C=%12C%25=C%13C%24=C%14C%23=C%15C%22=C%16C=%17C%21=C%18C=%19C=%20C%29C%21=C%22C(=C%23C%24=C%28C%25=C%26%27)C%29%30%31	228.0257611	36.000	40.663	-4.663
6	O=C(O)CCC%21(c1ccccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	224.3936598	10.000	14.757	-4.757
9	CC(O)OC(=O)CCC%21(c1ccccc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	225.4619958	22.000	22.377	-0.377
12	O=C(O)CCC%21(c1cccc(O)cc1)C%32%22C%31C=%19C=%33C=%17C%15=C5c4c%14c%13c%12c3c2c%11C%10=C8C=7C2=C(c34)C6=C5C=%33C%30=C6C=7C%29=C8C=%28C(C9=C%20C=%16C=%24C%27=C9C=%28C%10=C%26c%11c%12C%25=C%13C=%23C(=C%14%15)C%18=C(C=%16C(C=%19C=%17%18)C%20%21%22)C=%23C=%24C%25=C%26%27)=C%32C%29=C%30%31	223.8803115	5.000	11.096	-6.096
15	O=C(OCCC)CCC%37(c1ccccc1)C%32%38C4c%36c3c2c%34C%21=C%18c2c%14c%16c3C4=C%31C%17C%10=C%30C=%29C=9c8c%22c%24c7c5c%25c%27c%20c6c%19c%13c%12c(c56)c7c8C=%11C=9C%10=C%15C(C=%11%12)=C%13C(C%14=C%15C%16%17)=C%18C%19=C%20C%21=C%28C%35=C%33C%26=C%23C(=C(C=%29C%22=C%23c%24c%25C%26=C%27%28)C%32=C%30%31)C%37%38C%33c%36c%34%35	227.9541468	35.000	40.152	-5.152

18	O=C(OCCC)CCC%31(c1cccs1)C%28%30C%26C=%20C=%32C=%19C%33=C%10c3e9c2c8c7c6c5c2c4c3C%33=C%18C=%17C4=C5C%16=C%15C6=C%14C7=C%13C=%12C8=C9C%11=C%10C=%32C%27=C%11C=%12C%25=C%13C%24=C%14C%23=C%15C%22=C%16C=%17C%21=C%18C=%19C=%20C%29C%21=C%22C(=C%23C%24=C%28C%25=C%26%27)C%29%30%31	229.1993365	45.000	49.033	-4.033
21	O=C(OCCCC)CCC%38(c1cccs1)C%36%37C%28c%11c%27c2c%26C%23=C%34c2c%12C=%10C=%35C=9c%21c8c3c%20c%19c4c3c7c6c5c4C=%18C%17=C5C%16=C%15C6=C%13c7c8C=9C=%14C=%10C(c%11%12)C%37%38C(C%13=%14)=C%15C%36=C%29C%16=C%30C%17=C%33C=%25C=%18c%19c%24c%22c%20c%21C(=C%22C%23=C(C%24=%25)C=%32c%26c%31c%27C%28=C%29C%30C%31C=%32%33)C%34=%35	241.0801578	124.000	133.772	-9.772
24	CCCCCCC%31(c1cccs1)C%28%30C%26C=%20C=%32C=%19C%33=C%10c3e9c2c8c7c6c5c2c4c3C%33=C%18C=%17C4=C5C%16=C%15C6=C%14C7=C%13C=%12C8=C9C%11=C%10C=%32C%27=C%11C=%12C%25=C%13C%24=C%14C%23=C%15C%22=C%16C=%17C%21=C%18C=%19C=%20C%29C%21=C%22C(=C%23C%24=C%28C%25=C%26%27)C%29%30%31	229.3900328	25.000	50.394	-25.394
27	O=C(OCCCCCCC)C%24C%32%25C%16=C%14C%11=C%23C=%26C%13=C%20C3=C%12C=%10c2c9c8c1c7c6c5c4c1c2C3=C4C=%19C%18=C5C%17=C6C%27=C%29C7=C8C=%30C%15=C9C=%10C(C%11=C%12%13)=C%14C%15=C%31C%16=C%28C%32C=%22C(C%17=C%21C%18=C(C=%19%20)C=%26C(C%21=%22)C%23%24%25)=C%27C%28=C%29C=%30%31	220.8192013	9.000	-10.737	19.737

\*) Compound #5 is an outlier