

THREE DATASETS FROM THE PAPER “*MATRIX QUASI-NORMS AND NORMS AS MOLECULAR DESCRIPTORS*” BY PIOTR WILCZEK

QPSR studies on the molar refraction (MR) of aliphatic alcohols

$$MR = 3.6889(\pm 0.0848) + 2.3024(\pm 0.0061)\|A(G)\|_1 \quad (Eq. 7)$$

$$n = 41 \quad R^2 = 0.997 \quad s = 0.183 \quad F = 143210 \quad Q^2 = 0.9997 \quad SDEP = 0.1901$$

Table 1. The values of topological indices from Eq. 7

No.	Compound	$\ A(G)\ _1$
1	ethanol	4
2	propan-1-ol	6
3	propan-2-ol	6
4	butan-1-ol	8
5	2-methylpropan-1-ol	8
6	butan-2-ol	8
7	2-methylpropan-2-ol	8
8	pentan-1-ol	10
9	3-methylbutan-1-ol	10
10	pentan-2-ol	10
11	2-methylbutan-1-ol	10
12	pentan-3-ol	10
13	3-methylbutan-2-ol	10
14	2-methylbutan-2-ol	10
15	hexan-1-ol	12
16	2-methylpentan-1-ol	12
17	2-ethylbutan-1-ol	12
18	4-methylpentan-2-ol	12
19	2,3-dimethylbutan-2-ol	12
20	3,3-dimethylbutan-1-ol	12
21	3,3-dimethylbutan-2-ol	12
22	hexan-3ol	12
23	3-methylpentan-3-ol	12
24	heptan-1-ol	14
25	heptan-2-ol	14
26	heptan-3-ol	14
27	heptan-4-ol	14
28	2, 4-dimethylpentan-3-ol	14
29	octan-1-ol	16
30	octan-2-ol	16
31	octan-4-ol	16
32	2-ethylhexan-1-ol	16
33	2,2,4-trimethylpentan-1-ol	16
34	3,5-dimethylhexan-1-ol	16

35	nonan-1-ol	18
36	2,6-dimethylheptan-4-ol	18
37	nonan-5-ol	18
38	decan-1-ol	20
39	undecan-1-ol	22
40	2,6,8-trimethylnonan-4-ol	24
41	tridecan-1-ol	26

$$MR = -0.9159(\pm 0.0963) + 4.6048(\pm 0.0122)\|MM^2(G)\|_1 \quad (Eq. 8)$$

$$n = 41 \quad R^2 = 0.9997 \quad s = 0.183 \quad F = 143210 \quad Q^2 = 0.9997 \quad SDEP = 0.1901$$

Table 2. The values of topological indices from Eq. 8.

No.	Compound	$\ MM^2(G)\ _1$
1	ethanol	3
2	propan-1-ol	4
3	propan-2-ol	4
4	butan-1-ol	5
5	2-methylpropan-1-ol	5
6	butan-2-ol	5
7	2-methylpropan-2-ol	5
8	pentan-1-ol	6
9	3-methylbutan-1-ol	6
10	pentan-2-ol	6
11	2-methylbutan-1-ol	6
12	pentan-3-ol	6
13	3-methylbutan-2-ol	6
14	2-methylbutan-2-ol	6
15	hexan-1-ol	7
16	2-methylpentan-1-ol	7
17	2-ethylbutan-1-ol	7
18	4-methylpentan-2-ol	7
19	2,3-dimethylbutan-2-ol	7
20	3,3-dimethylbutan-1-ol	7
21	3,3-dimethylbutan-2-ol	7
22	hexan-3-ol	7
23	3-methylpentan-3-ol	7
24	heptan-1-ol	8
25	heptan-2-ol	8
26	heptan-3-ol	8
27	heptan-4-ol	8
28	2, 4-dimethylpentan-3-ol	8
29	octan-1-ol	9
30	octan-2-ol	9
31	octan-4-ol	9
32	2-ethylhexan-1-ol	9
33	2,2,4-trimethylpentan-1-ol	9
34	3,5-dimethylhexan-1-ol	9

35	nonan-1-ol	10
36	2,6-dimethylheptan-4-ol	10
37	nonan-5-ol	10
38	decan-1-ol	11
39	undecan-1-ol	12
40	2,6,8-trimethylnonan-4-ol	13
41	tridecan-1-ol	14

$$MR = 33.9009(\pm 0.0285) + 68.6648(\pm 0.1826)\|A(G)\|_{1.975}^{Sch} + 8.911(\pm 0.1826)(\|A(G)\|_{1.975}^{Sch})^2 \quad (Eq. 9)$$

$$n = 41 \quad R^2 = 0.9997 \quad s = 0.1826 \quad F = 71909.91 \quad Q^2 = 0.9997 \quad SDEP = 0.2015$$

Table 3. The values of topological indices from Eq. 9.

No.	Compound	$\ A(G)\ _{1.975}^{Sch}$
1	ethanol	2.0088
2	propan-1-ol	2.4662
3	propan-2-ol	2.4603
4	butan-1-ol	2.8510
5	2-methylpropan-1-ol	2.8484
6	butan-2-ol	2.8484
7	2-methylpropan-2-ol	2.8409
8	pentan-1-ol	3.1918
9	3-methylbutan-1-ol	3.1881
10	pentan-2-ol	3.1881
11	2-methylbutan-1-ol	3.1903
12	pentan-3-ol	3.1903
13	3-methylbutan-2-ol	3.1863
14	2-methylbutan-2-ol	3.1844
15	hexan-1-ol	3.4996
16	2-methylpentan-1-ol	3.4978
17	2-ethylbutan-1-ol	3.4985
18	4-methylpentan-2-ol	3.4934
19	2,3-dimethylbutan-2-ol	3.4907
20	3,3-dimethylbutan-1-ol	3.4921
21	3,3-dimethylbutan-2-ol	3.4907
22	hexan-3-ol	3.4978
23	3-methylpentan-3-ol	3.4948
24	heptan-1-ol	3.7834
25	heptan-2-ol	3.7805
26	heptan-3-ol	3.7821
27	heptan-4-ol	3.7809
28	2, 4-dimethylpentan-3-ol	3.7775
29	octan-1-ol	4.0476
30	octan-2-ol	4.0453
31	octan-4-ol	4.0458
32	2-ethylhexan-1-ol	4.0466
33	2,2,4-trimethylpentan-1-ol	4.0399
34	3,5-dimethylhexan-1-ol	4.0427

35	nonan-1-ol	4.2961
36	2,6-dimethylheptan-4-ol	4.2890
37	nonan-5-ol	4.2948
38	decan-1-ol	4.5312
39	undecan-1-ol	4.7551
40	2,6,8-trimethylnonan-4-ol	4.9612
41	tridecan-1-ol	5.1744