*J. Braz. Chem. Soc.*, Vol. 24, No. 11, S1-S5, 2013.
Printed in Brazil - ©2013 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

# Supplementary Information

## QSAR Models of Reaction Rate Constants of Alkenes with Ozone and Hydroxyl Radical

***Yueyu Xu,[a] Xinliang Yu*,[a] and Shihua Zhang*,[a,b]***

*[a]College of Chemistry and Chemical Engineering, [b]Network Information Center, Hunan Institute of Engineering, Xiangtan, Hunan 411104, China*

**Table S1.** Quantum chemical descriptors and -log$k_{O3}$ values for 95 alkenes[a]

| No. | Name | $E_{GHOMO}$ / a.u. | $q_{IC12}$ / a.u. | $Q_{IO12}$ / a.u. | -log$k_{O3}$ (exp.) | -log$k_{O3}$ (pred.)[b] | -log$k_{O3}$ (pred.)[c] |
|---|---|---|---|---|---|---|---|
| | | | Training set | | | | |
| 1 | 1,3-Cyclohexadiene | -0.205526 | 0.687946 | -0.608815 | 14.7 | 14.44 | 14.93 |
| 2 | Bicyclo(2.2.1)-2-heptene | -0.230909 | 0.539394 | -0.603226 | 14.7 | 15.49 | 14.86 |
| 3 | 1,3-Cycloheptadiene | -0.208367 | 0.726131 | -0.599350 | 15.8 | 14.71 | 15.55 |
| 4 | Carvomenthene | -0.230995 | 0.712092 | -0.565545 | 15.3 | 16.09 | 15.82 |
| 5 | Terpinolene | -0.215923 | 0.683347 | -0.615165 | 14 | 14.81 | 14.06 |
| 6 | Tetrafluoroethene | -0.254209 | 2.531489 | -0.530281 | 19 | 19.01 | 19.00 |
| 7 | 1,1-dichloroethene | -0.266297 | 1.353019 | -0.453706 | 20.4 | 19.51 | 20.31 |
| 8 | 2-methyl-1-butene | -0.239266 | 0.688732 | -0.553380 | 16.8 | 16.58 | 16.48 |
| 9 | Hexafluoropropene | -0.281063 | 1.928487 | -0.532637 | 19.1 | 19.66 | 19.10 |
| 10 | 2-(chloromethyl)-3-chloro-1-propene | -0.277909 | 0.622758 | -0.539928 | 18.4 | 18.38 | 18.40 |
| 11 | 1.2-Propadiene | -0.262966 | 0.788560 | -0.561417 | 18.72 | 17.60 | 18.72 |
| 12 | 1-Methyl-1-cyclopentene | -0.223285 | 0.689486 | -0.590023 | 15.17 | 15.44 | 15.40 |
| 13 | 2-Methyl-1.4-pentadiene | -0.241725 | 0.684857 | -0.537600 | 16.89 | 16.88 | 16.94 |
| 14 | 1.2-Dimethylcyclohexene | -0.216046 | 0.690035 | -0.591053 | 15.68 | 15.11 | 15.44 |
| 15 | *Trans*-3-Hexene | -0.235597 | 0.681452 | -0.556782 | 15.77 | 16.38 | 16.09 |
| 16 | 3-methyl-1-butene | -0.249284 | 0.692447 | -0.530566 | 16.96 | 17.30 | 16.99 |
| 17 | *Trans*-2,5-Dimethyl-3-hexene | -0.235390 | 0.658580 | -0.566235 | 16.39 | 16.23 | 16.06 |
| 18 | *Cis*- +trans-3,4-Dimethyl-3-hexene | -0.215528 | 0.709946 | -0.592469 | 15.42 | 15.09 | 15.44 |
| 19 | *Cis*-Cyclooctene | -0.231456 | 0.726928 | -0.558084 | 15.43 | 16.22 | 15.87 |
| 20 | Propene | -0.249793 | 0.721658 | -0.524060 | 16.9 | 17.43 | 16.95 |
| 21 | *Cis*-2-Butene | -0.233323 | 0.762977 | -0.561473 | 15.8 | 16.29 | 15.91 |
| 22 | 1-Pentene | -0.246525 | 0.709157 | -0.531907 | 17 | 17.18 | 16.98 |
| 23 | *Trans*-2-Pentene | -0.230672 | 0.711240 | -0.555324 | 15.5 | 16.20 | 15.87 |
| 24 | 1-Hexene | -0.246307 | 0.708191 | -0.532102 | 16.9 | 17.17 | 16.98 |
| 25 | 2-Methyl-1-pentene | -0.238959 | 0.703121 | -0.542675 | 16.8 | 16.71 | 16.77 |
| 26 | *Trans*-3-Methyl-2-pentene | -0.217403 | 0.707823 | -0.592823 | 15.2 | 15.17 | 15.41 |
| 27 | 2-Heptene | -0.230412 | 0.711206 | -0.560874 | 16.1 | 16.12 | 15.83 |
| 28 | β-Pinene | -0.233026 | 0.654833 | -0.576236 | 16.5 | 16.01 | 16.15 |
| 29 | β-Phellandrene | -0.213644 | 0.708764 | -0.557507 | 15.7 | 15.43 | 15.76 |
| 30 | *Trans*-cyclooctene | -0.231075 | 0.726928 | -0.558084 | 16.54 | 16.20 | 15.86 |
| 31 | 2,4,4-trimethyl-2-pentene | -0.226734 | 0.705376 | -0.587445 | 15.85 | 15.64 | 15.59 |
| 32 | *Trans*-5-decene | -0.229245 | 0.689435 | -0.564497 | 15.89 | 16.01 | 15.79 |
| 33 | 1-Methyl-1-cyclohexene | -0.224367 | 0.687781 | -0.570094 | 15.78 | 15.73 | 15.61 |
| 34 | 2.5-Dimethyl-1.5-hexadiene | -0.235703 | 0.728943 | -0.557431 | 16.85 | 16.41 | 16.09 |
| 35 | 1-Octene | -0.246141 | 0.726278 | -0.546258 | 17.1 | 17.00 | 17.07 |
| 36 | 1,3-Butadiene | -0.228950 | 0.757909 | -0.521879 | 17.1 | 16.57 | 16.80 |
| 37 | Dihydromyrcene | -0.225079 | 0.698931 | -0.530083 | 15.2 | 16.26 | 15.93 |

*e-mail: yxliang5602@sina.com.cn, shihua_zh@sina.cn

**Table S1.** continuation

| No. | Name | $E_{GHOMO}$ / a.u. | $q_{IC12}$ / a.u. | $Q_{IO12}$ / a.u. | -log$k_{O3}$ (exp.) | -log$k_{O3}$ (pred.)[b] | -log$k_{O3}$ (pred.)[c] |
|---|---|---|---|---|---|---|---|
| | | | Training set | | | | |
| 38 | *Cis*-Ocimene | -0.219579 | 0.719544 | -0.528799 | 14.7 | 16.05 | 15.04 |
| 39 | α-Terpinene | -0.192386 | 0.696624 | -0.636419 | 13.1 | 13.54 | 13.10 |
| 40 | 1,1-Difluoroethene | -0.262252 | 1.613112 | -0.527680 | 18.7 | 18.65 | 18.70 |
| 41 | *Cis*-1,3-dichloropropene | -0.266567 | 0.951379 | -0.479781 | 18.8 | 18.88 | 18.79 |
| 42 | Acrolein | -0.257123 | 0.558858 | -0.487809 | 18.3 | 18.06 | 18.30 |
| 43 | Methyl vinyl ketone | -0.247851 | 0.547462 | -0.558508 | 17.4 | 16.78 | 17.39 |
| 44 | 2-cyclohexen-1-one | -0.236331 | 0.578369 | -0.519273 | 17.7 | 16.78 | 17.69 |
| 45 | 3.3-Dimethyl-1-butene | -0.249533 | 0.662849 | -0.539712 | 17.28 | 17.18 | 17.10 |
| 46 | *Cis*-5-Decene | -0.231212 | 0.722127 | -0.563115 | 15.92 | 16.14 | 15.84 |
| 47 | *Cis*-3-Hexene | -0.231830 | 0.710888 | -0.561279 | 15.82 | 16.18 | 15.86 |
| 48 | Ethene | -0.266547 | 0.702671 | -0.504672 | 17.7 | 18.38 | 17.70 |
| 49 | 2.3-Dimethyl-1.3-butadiene | -0.224837 | 0.690641 | -0.548631 | 16.58 | 16.01 | 16.29 |
| 50 | 2-methyl-1,3-butadiene | -0.226117 | 0.696111 | -0.525793 | 16.89 | 16.35 | 16.24 |
| 51 | *Cis*-2,*trans*-4-Hexadiene | -0.208020 | 0.773115 | -0.549613 | 15.5 | 15.34 | 15.67 |
| 52 | Cycloheptene | -0.230329 | 0.701853 | -0.562377 | 15.5 | 16.10 | 15.82 |
| 53 | 1,4-Cyclohexadiene | -0.226180 | 0.653269 | -0.611527 | 16.2 | 15.28 | 16.08 |
| 54 | Bicyclo(2.2.2)-2-octene | -0.234554 | 0.703257 | -0.600302 | 16.1 | 15.82 | 16.03 |
| 55 | 1,3,5-Cycloheptatriene | -0.212641 | 0.746006 | -0.544032 | 16.3 | 15.58 | 16.07 |
| 56 | *d*-Limonene | -0.225634 | 0.715009 | -0.574389 | 15.2 | 15.75 | 15.56 |
| 57 | Trifluoroethene | -0.254416 | 2.080157 | -0.533009 | 18.9 | 18.62 | 18.90 |
| 58 | Methacrolein | -0.255129 | 0.558435 | -0.517032 | 18 | 17.61 | 17.97 |
| 59 | Vinyl chloride | -0.262460 | 1.064558 | -0.470593 | 18.6 | 18.91 | 18.61 |
| 60 | *Cis*-1,2-dichloroethene | -0.259607 | 1.323410 | -0.446518 | 19.2 | 19.29 | 19.29 |
| | | | Test set | | | | |
| 61 | Trichloroethene | -0.261331 | 1.615179 | -0.431117 | 19.5 | 19.79 | 19.33 |
| 62 | Octafluoro-2-butene | -0.303156 | 1.409374 | -0.534576 | 20.2 | 20.18 | 19.10 |
| 63 | Cyclopentene | -0.232844 | 0.693015 | -0.564597 | 15.56 | 16.17 | 15.89 |
| 64 | 2.3-Dimethyl-2-butene | -0.217788 | 0.749722 | -0.580553 | 14.82 | 15.37 | 15.43 |
| 65 | 2-Ethylbutene | -0.238800 | 0.682848 | -0.553128 | 16.89 | 16.56 | 16.44 |
| 66 | 2.4-Dimethyl-1.3-butadiene | -0.215685 | 0.795419 | -0.538723 | 16.1 | 15.82 | 15.91 |
| 67 | *Trans*-4-Octene | -0.234244 | 0.696825 | -0.560270 | 15.85 | 16.29 | 15.97 |
| 68 | 3-methyl-1-pentene | -0.248993 | 0.699206 | -0.535291 | 17.31 | 17.24 | 17.03 |
| 69 | *Trans*-2,2-Dimethyl-3-hexene | -0.235538 | 0.651240 | -0.601851 | 16.38 | 15.80 | 15.89 |
| 70 | 1,3,5-Hexatriene | -0.209225 | 0.751076 | -0.536485 | 16.6 | 15.53 | 16.02 |
| 71 | 2-Methyl-2-propene | -0.239539 | 0.717789 | -0.545965 | 16.9 | 16.71 | 16.71 |
| 72 | *Trans*-2-Butene | -0.235027 | 0.740022 | -0.550173 | 15.6 | 16.48 | 16.12 |
| 73 | *cis*-2-Pentene | -0.232569 | 0.723065 | -0.543939 | 15.7 | 16.43 | 16.00 |
| 74 | 2-Methyl-2-butene | -0.225635 | 0.748689 | -0.578196 | 15.4 | 15.74 | 15.51 |
| 75 | 4-Methyl-1-pentene | -0.249099 | 0.705650 | -0.522110 | 17 | 17.41 | 16.95 |
| 76 | *Cis*-3-Methyl-2-pentene | -0.224347 | 0.734981 | -0.566204 | 15.3 | 15.81 | 15.67 |
| 77 | 1-Heptene | -0.246201 | 0.707874 | -0.532087 | 16.9 | 17.16 | 16.98 |
| 78 | α-Pinene | -0.218341 | 0.770965 | -0.591064 | 15.7 | 15.28 | 15.39 |
| 79 | D3-Carene | -0.224523 | 1.025169 | -0.532474 | 15.9 | 16.47 | 16.33 |
| 80 | γ-Terpinene | -0.217922 | 0.685046 | -0.580884 | 15.6 | 15.32 | 15.44 |
| 81 | 3-methyl-2-isopropyl-1-butene | -0.237362 | 0.622156 | -0.560336 | 17.48 | 16.36 | 16.20 |
| 82 | 4-Methyl-1-cyclohexene | -0.233595 | 0.688425 | -0.555796 | 16.09 | 16.31 | 15.96 |
| 83 | 2.3.3.-Trimethylbutene | -0.239373 | 0.647121 | -0.559572 | 17.08 | 16.48 | 16.37 |
| 84 | 1-Butene | -0.246661 | 0.707276 | -0.521192 | 16.9 | 17.31 | 16.94 |
| 85 | 1-Decene | -0.246066 | 0.712919 | -0.522230 | 17 | 17.28 | 16.94 |
| 86 | Myrcene | -0.222559 | 0.699391 | -0.530152 | 14.9 | 16.15 | 15.53 |
| 87 | Vinyl fluoride | -0.260366 | 1.174156 | -0.532133 | 18.2 | 18.15 | 18.70 |
| 88 | *Trans*-1,2-dichloroethene | -0.259885 | 1.295515 | -0.474002 | 18.7 | 18.94 | 19.10 |

**Table S1.** continuation

| No. | Name | $E_{GHOMO}$ / a.u. | $q_{IC12}$ / a.u. | $Q_{IO12}$ / a.u. | -log$k_{O3}$ (exp.) | -log$k_{O3}$ (pred.)[b] | -log$k_{O3}$ (pred.)[c] |
|---|---|---|---|---|---|---|---|
| | | | Test set | | | | |
| 89 | *Cis*-1,2-difluoroethene | -0.254139 | 1.645013 | -0.523658 | 18.6 | 18.37 | 18.70 |
| 90 | Trans-1,3-dichloropropene | -0.262766 | 1.039316 | -0.457231 | 18.2 | 19.06 | 18.60 |
| 91 | 2.3-Dimethyl-1-butene | -0.239239 | 0.669720 | -0.558808 | 16.89 | 16.50 | 16.37 |
| 92 | 3-penten-2-one | -0.240713 | 0.554961 | -0.538358 | 16.7 | 16.72 | 16.94 |
| 93 | *Cis*-4-Octene | -0.233860 | 0.714750 | -0.546147 | 16.02 | 16.46 | 16.06 |
| 94 | Trans-2,trans-4-Hexadiene | -0.207551 | 0.781737 | -0.562995 | 15.4 | 15.16 | 15.59 |
| 95 | Cyclohexene | -0.233459 | 0.706416 | -0.545016 | 15.9 | 16.45 | 16.04 |

[a]Experimental data taken from: Yu, X.; Yi, B.; Wang, X.; Chen, J.; *Atmos. Environ.* **2012**, *51*, 124; [b]-log$k_{O3}$ values predicted from the MLR model for -log$k_{O3}$; [c]-log$k_{O3}$ values predicted from the GRNN model for -log$k_{O3}$.

**Table S2.** Quantum chemical descriptors and -log$k_{OH}$ values for 98 alkenes[a]

| No. | Name | $\mu_l$ / Debye. | $E_{I\beta HOMO}$ / a.u. | $E_{GHOMO}$ / a.u. | $Q_{IC12}$ / a.u. | -log$k_{OH}$ (exp.) | -log$k_{OH}$ (pred.)[b] | -log$k_{OH}$ (pred.)[c] |
|---|---|---|---|---|---|---|---|---|
| | | | | Training set | | | | |
| 1 | α-Phellandrene | 1.4824 | -0.231877 | -0.201328 | 0.386365 | 9.5 | 9.64 | 9.54 |
| 2 | Ocimene | 1.7247 | -0.223650 | -0.214890 | 0.348628 | 9.6 | 9.72 | 9.75 |
| 3 | α-Humulene | 0.8406 | -0.219121 | -0.216163 | 0.306492 | 9.65 | 9.86 | 9.65 |
| 4 | Myrcene | 2.0283 | -0.227171 | -0.222559 | 0.337243 | 9.67 | 9.78 | 9.74 |
| 5 | 3-7-Dimethyl-1-6-Octadiene | 1.7370 | -0.227728 | -0.223194 | 0.337042 | 9.74 | 9.86 | 9.77 |
| 6 | β-Phellandrene | 1.4332 | -0.251327 | -0.213643 | 0.379030 | 9.78 | 9.92 | 9.91 |
| 7 | 2-4-Dimethyl-1-3-butadiene | 1.5318 | -0.241135 | -0.214725 | 0.378989 | 9.8 | 9.87 | 9.88 |
| 8 | Limonene | 1.8410 | -0.223396 | -0.225634 | 0.370411 | 9.84 | 9.90 | 9.80 |
| 9 | 3-Methyl-1-3-Pentadiene | 1.5915 | -0.231610 | -0.213908 | 0.340018 | 9.87 | 9.76 | 9.85 |
| 10 | *Trans-trans*-2-4-Hexadiene | 1.6603 | -0.242251 | -0.205513 | 0.425635 | 9.87 | 9.76 | 9.88 |
| 11 | *Trans*-3-Methyl-2-Pentene | 1.5760 | -0.263403 | -0.217403 | 0.396933 | 9.91 | 10.02 | 9.98 |
| 12 | 2-5-Norbornadiene | 1.4479 | -0.234600 | -0.216970 | 0.296089 | 9.92 | 9.80 | 9.89 |
| 13 | 1-2-Dimethylcyclohexene | 1.2055 | -0.254068 | -0.216046 | 0.512535 | 9.93 | 10.19 | 9.93 |
| 14 | Trans-1-3-5-Hexatriene | 1.5081 | -0.246912 | -0.209238 | 0.377880 | 9.95 | 9.81 | 9.92 |
| 15 | *Cis*-1-3-5-Hexatriene | 1.5697 | -0.227117 | -0.209994 | 0.377086 | 9.96 | 9.73 | 9.87 |
| 16 | *Cis*-Ocimene | 1.8549 | -0.219184 | -0.219579 | 0.312578 | 9.98 | 9.70 | 9.86 |
| 17 | 2-carene | 1.3670 | -0.249451 | -0.214811 | 0.364724 | 10 | 9.93 | 9.91 |
| 18 | *Cis*-1-3-Pentadiene | 1.7194 | -0.260118 | -0.218090 | 0.396585 | 10 | 9.99 | 10.03 |
| 19 | 1-3-5-Cycloheptatriene | 1.5436 | -0.246124 | -0.212641 | 0.450317 | 10.01 | 9.95 | 9.94 |
| 20 | 2-Methyl-1-5-Hexadiene | 1.2764 | -0.243735 | -0.241347 | 0.319746 | 10.02 | 10.30 | 10.02 |
| 21 | *Cis*-3-Methyl-2-Pentene | 1.4481 | -0.260926 | -0.224349 | 0.420357 | 10.03 | 10.18 | 10.05 |
| 22 | 1-Methyl-1-Cyclopentene | 1.4843 | -0.256565 | -0.223283 | 0.407197 | 10.04 | 10.12 | 10.05 |
| 23 | 2-Ethylbutene | 1.5531 | -0.265850 | -0.238794 | 0.305473 | 10.05 | 10.27 | 10.21 |
| 24 | D3-Carene | 1.7846 | -0.244998 | -0.224523 | 0.394391 | 10.06 | 10.01 | 10.07 |
| 25 | *Trans*-3-Hexene | 1.5012 | -0.263229 | -0.229750 | 0.326852 | 10.08 | 10.15 | 10.16 |
| 26 | *Cis*-5-Decene | 1.7345 | -0.260888 | -0.231210 | 0.341035 | 10.12 | 10.13 | 10.18 |
| 27 | *Cis*-3-Hexene | 1.5511 | -0.260855 | -0.231830 | 0.315984 | 10.13 | 10.15 | 10.18 |
| 28 | Methylketene | 4.3775 | -0.268694 | -0.222801 | 0.998893 | 10.16 | 10.29 | 10.16 |
| 29 | 1,3-butadiene | 1.6159 | -0.258498 | -0.228950 | 0.357837 | 10.17 | 10.13 | 10.17 |
| 30 | Cyclopentene | 1.4046 | -0.258164 | -0.232844 | 0.343862 | 10.17 | 10.22 | 10.20 |
| 31 | Trans-2-heptene | 1.6931 | -0.259383 | -0.230412 | 0.341409 | 10.17 | 10.12 | 10.18 |
| 32 | 2-methyl-1-pentene | 1.4380 | -0.264791 | -0.238959 | 0.344140 | 10.2 | 10.34 | 10.21 |
| 33 | 1,5-hexadiene | 1.8494 | -0.251802 | -0.249422 | 0.338346 | 10.21 | 10.36 | 10.32 |
| 34 | 4-methyl-1-cyclohexene | 1.3811 | -0.256752 | -0.233595 | 0.390818 | 10.21 | 10.29 | 10.23 |
| 35 | 3-methyl-1,2-butadiene | 1.8010 | -0.234038 | -0.235227 | 0.276072 | 10.24 | 9.99 | 10.24 |

**Table S2.** continuation

| No. | Name | $\mu_I$ / Debye. | $E_{I\beta HOMO}$ / a.u. | $E_{GHOMO}$ / a.u. | $Q_{IC12}$ / a.u. | -log$k_{OH}$ (exp.) | -log$k_{OH}$ (pred.)[b] | -log$k_{OH}$ (pred.)[c] |
|---|---|---|---|---|---|---|---|---|
| | | | | Training set | | | | |
| 36 | α-pinene | 1.7989 | -0.254171 | -0.218341 | 0.393235 | 10.26 | 9.95 | 10.11 |
| 37 | *Cis*-2-butene | 1.7860 | -0.262610 | -0.233323 | 0.408649 | 10.26 | 10.25 | 10.21 |
| 38 | Camphene | 1.4010 | -0.263749 | -0.233314 | 0.272334 | 10.27 | 10.17 | 10.19 |
| 39 | 2,3-dimethyl-1-butene | 1.6013 | -0.266191 | -0.239239 | 0.314830 | 10.28 | 10.28 | 10.21 |
| 40 | 2,3,3-trimethylbutene | 1.6417 | -0.263018 | -0.239358 | 0.328902 | 10.3 | 10.28 | 10.23 |
| 41 | Cis-Cyclooctene | 1.6066 | -0.253752 | -0.231830 | 0.347259 | 10.38 | 10.15 | 10.22 |
| 42 | Bicycle(2, 2, 2)-2-Octene | 1.4061 | -0.255391 | -0.234580 | 0.460586 | 10.39 | 10.38 | 10.30 |
| 43 | 4-methyl-1-pentene | 1.5886 | -0.262981 | -0.249101 | 0.338715 | 10.42 | 10.46 | 10.46 |
| 44 | 1-Decene | 1.8493 | -0.258003 | -0.246066 | 0.335645 | 10.43 | 10.33 | 10.42 |
| 45 | 1-Butene | 1.8309 | -0.259331 | -0.246661 | 0.324568 | 10.5 | 10.34 | 10.43 |
| 46 | 3,3-Dimethyl-1-Butene | 1.5682 | -0.263495 | -0.249531 | 0.304249 | 10.55 | 10.43 | 10.47 |
| 47 | *Cis*-1,3-Dichloroperopene | 3.2949 | -0.294107 | -0.266567 | 0.944536 | 11.08 | 11.27 | 11.08 |
| 48 | 1-Chloroethene | 1.9759 | -0.279475 | -0.262491 | 0.632896 | 11.18 | 11.03 | 11.18 |
| 49 | *Cis*-1,2-Difluoroethene | 1.8755 | -0.314502 | -0.254139 | 1.325095 | 12.15 | 11.94 | 12.15 |
| | | | | Test set | | | | |
| 50 | α-Terpinene | 2.0858 | -0.232670 | -0.192386 | 0.435730 | 9.44 | 9.43 | 9.54 |
| 51 | *Trans*-Ocimene | 1.7246 | -0.223649 | -0.214890 | 0.348622 | 9.6 | 9.72 | 9.75 |
| 52 | Terpinolene | 1.3946 | -0.228190 | -0.215923 | 0.490789 | 9.65 | 10.01 | 9.86 |
| 53 | 1-3-5-Hexatriene | 1.5081 | -0.246912 | -0.209238 | 0.377880 | 9.66 | 9.81 | 9.92 |
| 54 | 2-5-Dimethyl-2-4-Hexadiene | 1.9270 | -0.235355 | -0.194584 | 0.439269 | 9.68 | 9.51 | 9.58 |
| 55 | γ-Terpinene | 1.7112 | -0.232884 | -0.217922 | 0.401595 | 9.75 | 9.88 | 9.81 |
| 56 | 1-3-Cyclohexadiene | 2.2179 | -0.243968 | -0.205526 | 0.411646 | 9.79 | 9.63 | 9.88 |
| 57 | *Cis*-2-trans-4-Hexadiene | 1.3842 | -0.238352 | -0.207100 | 0.424245 | 9.81 | 9.83 | 9.85 |
| 58 | 1-3-Cycloheptadiene | 1.6743 | -0.233355 | -0.216948 | 0.337400 | 9.86 | 9.79 | 9.84 |
| 59 | 4-Methyl-1-3-Pentadiene | 1.6156 | -0.233286 | -0.207910 | 0.359410 | 9.88 | 9.69 | 9.84 |
| 60 | 2-3-Dimethyl-1-3-Butadiene | 1.8076 | -0.248685 | -0.224837 | 0.372377 | 9.91 | 10.00 | 10.11 |
| 61 | β-Caryophyllene | 1.2463 | -0.221001 | -0.219970 | 0.304256 | 9.92 | 9.84 | 9.74 |
| 62 | 2-5-Dimethyl-1-5-Hexadiene | 1.8965 | -0.238133 | -0.233258 | 0.350638 | 9.92 | 10.05 | 10.21 |
| 63 | *Trans*-1-3-Hexadiene | 1.8150 | -0.264811 | -0.215871 | 0.359915 | 9.95 | 9.91 | 10.00 |
| 64 | 2-3-Dimethyl-2-Butene | 1.4108 | -0.259953 | -0.217816 | 0.516044 | 9.96 | 10.20 | 9.96 |
| 65 | Dimethylketene | 4.7987 | -0.261749 | -0.211921 | 1.031781 | 9.97 | 10.03 | 10.16 |
| 66 | 2-Methyl-1-3-Butadiene | 1.3600 | -0.258270 | -0.226117 | 0.348285 | 10 | 10.13 | 10.12 |
| 67 | 1-4-Cyclohexadiene | 1.5143 | -0.236744 | -0.226180 | 0.330141 | 10 | 9.98 | 9.90 |
| 68 | *Trans*-1-3-Pentadiene | 1.5856 | -0.263320 | -0.216601 | 0.311442 | 10 | 9.90 | 9.97 |
| 69 | 2-3-Dimethyl-2-Pentene | 1.5624 | -0.258862 | -0.211185 | 0.464335 | 10.01 | 9.99 | 9.94 |
| 70 | 1-Methylcyclohexene | 1.2382 | -0.254919 | -0.224366 | 0.418505 | 10.03 | 10.20 | 10.05 |
| 71 | 2-Methyl-2-Pentene | 1.5670 | -0.263738 | -0.221978 | 0.403204 | 10.04 | 10.11 | 10.01 |
| 72 | *Trans*-1-4-Hexadiene | 1.8623 | -0.240840 | -0.230689 | 0.343403 | 10.04 | 10.01 | 10.15 |
| 73 | 2-Methyl-2-Butene | 1.7199 | -0.255803 | -0.225635 | 0.412442 | 10.06 | 10.11 | 10.12 |
| 74 | 2-Heptene | 1.6930 | -0.259383 | -0.230412 | 0.341406 | 10.07 | 10.12 | 10.18 |
| 75 | 2-Methyl-1-4-Pentadiene | 1.3669 | -0.243179 | -0.239354 | 0.339253 | 10.1 | 10.27 | 10.04 |
| 76 | Cycloheptene | 1.4482 | -0.256849 | -0.232142 | 0.381290 | 10.13 | 10.24 | 10.21 |
| 77 | *Cis*-4-octene | 1.3845 | -0.261839 | -0.231550 | 0.312938 | 10.14 | 10.18 | 10.17 |
| 78 | *Trans*-4-octene | 1.6524 | -0.258211 | -0.229560 | 0.398424 | 10.16 | 10.18 | 10.18 |
| 79 | Cyclohexene | 1.7324 | -0.255118 | -0.233459 | 0.329525 | 10.17 | 10.13 | 10.22 |
| 80 | *Trans*-2-pentene | 1.4261 | -0.262505 | -0.230681 | 0.334536 | 10.17 | 10.19 | 10.16 |
| 81 | *Cis*-2-pentene | 1.6360 | -0.259237 | -0.232569 | 0.396460 | 10.18 | 10.24 | 10.21 |
| 82 | *Trans*-2-butene | 1.6587 | -0.260163 | -0.235027 | 0.361226 | 10.22 | 10.23 | 10.21 |
| 83 | 2-methyl-1-butene | 1.4756 | -0.265263 | -0.239266 | 0.333624 | 10.22 | 10.33 | 10.21 |
| 84 | *Trans*-4-methyl-2-pentene | 1.4187 | -0.259956 | -0.235456 | 0.378799 | 10.22 | 10.31 | 10.21 |
| 85 | Sabinene | 1.9228 | -0.254161 | -0.221302 | 0.396345 | 10.25 | 9.97 | 10.14 |
| 86 | 2-methyl-1-propene | 1.5207 | -0.265485 | -0.239567 | 0.359728 | 10.26 | 10.36 | 10.22 |

**Table S2.** continuation

| No. | Name | $\mu_I$ / Debye. | $E_{I\beta HOMO}$ / a.u. | $E_{GHOMO}$ / a.u. | $Q_{IC12}$ / a.u. | -log$k_{OH}$ (exp.) | -log$k_{OH}$ (pred.)[b] | -log$k_{OH}$ (pred.)[c] |
|---|---|---|---|---|---|---|---|---|
| | | | | Test set | | | | |
| 87 | *Trans*-4,4-dimethyl-2-pentene | 1.5498 | -0.260832 | -0.232897 | 0.293190 | 10.26 | 10.14 | 10.18 |
| 88 | 1,4-Pentadiene | 1.7022 | -0.252850 | -0.240502 | 0.307939 | 10.27 | 10.21 | 10.31 |
| 89 | Bicycle(2, 2, 1)-2-heptene | 1.5115 | -0.258902 | -0.230925 | 0.305581 | 10.31 | 10.12 | 10.18 |
| 90 | Longifolene | 1.5343 | -0.258575 | -0.229710 | 0.287896 | 10.35 | 10.08 | 10.17 |
| 91 | 1-Heptene | 1.8080 | -0.261668 | -0.246201 | 0.315476 | 10.39 | 10.33 | 10.43 |
| 92 | 1-Octene | 1.5705 | -0.262658 | -0.246141 | 0.326022 | 10.4 | 10.40 | 10.41 |
| 93 | 1-Hexene | 1.8387 | -0.258431 | -0.246307 | 0.335618 | 10.43 | 10.34 | 10.42 |
| 94 | 3-methyl-1-Butene | 1.7204 | -0.260006 | -0.249824 | 0.309133 | 10.49 | 10.39 | 10.45 |
| 95 | 1-Pentene | 1.8387 | -0.258858 | -0.246525 | 0.335080 | 10.5 | 10.34 | 10.42 |
| 96 | Ketene | 2.5412 | -0.303842 | -0.240468 | 0.703868 | 10.76 | 10.75 | 11.18 |
| 97 | 1-Bromoethene | 1.8529 | -0.276904 | -0.254441 | 0.577348 | 11.17 | 10.85 | 11.18 |
| 98 | *Trans*-1,2-Difluoroethene | 1.4297 | -0.322054 | -0.253777 | 1.301103 | 12.13 | 12.03 | 12.15 |

[a]Experimental data taken from: Fatemi, M. H.; Baher, E.; *SAR QSAR Environ. Res.* **2009**, *20*, 77; [b]-log$k_{OH}$ values predicted from the MLR model for -log$k_{OH}$; [c]-log$k_{OH}$ values predicted from the GRNN model for -log$k_{OH}$.