**SUPPLEMENTARY MATERIAL**

A Robust Model for Estimating Thermal Conductivity of Liquid Halogenated Alkanes

Haixia Lua, Fan Yanga, Wanqiang Liua,b, Hua Yuana,b, Yinchun Jiaoa,b

**Corresponding Author:** E-mail: wanqiangliu@hnust.edu.cn

[yinchunjiao@hnust.edu.cn](mailto:yinchunjiao@hnust.edu.cn)

Table S1. Experiment and calculated values of thermal conductivity for training set and prediction set

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Set** | **No.** | **Compound** | **Formula** | ***B02*[*F-F*]** | ***T*** | ***SM3\_B*(*m*)** | ***SpMax\_AEA*(*ri*)** | ***RPCG*** | ***Mor11v*** | ***λ*exp/**  **(W/m·K)** | **GFA-MLR-*λ*cal/**  **(W/m·K)** |
| **Training set** | 1 | Carbon tetrachloride | CCl4 | 0.000 | 260 | 5.089 | 0.850 | 0.250 | -0.307 | 0.112 | 0.106 |
|  | 2 | Carbon tetrachloride | CCl4 | 0.000 | 270 | 5.089 | 0.850 | 0.250 | -0.307 | 0.109 | 0.105 |
|  | 3 | Carbon tetrachloride | CCl4 | 0.000 | 280 | 5.089 | 0.850 | 0.250 | -0.307 | 0.107 | 0.103 |
|  | 4 | Carbon tetrachloride | CCl4 | 0.000 | 290 | 5.089 | 0.850 | 0.250 | -0.307 | 0.105 | 0.101 |
|  | 5 | Carbon tetrachloride | CCl4 | 0.000 | 300 | 5.089 | 0.850 | 0.250 | -0.307 | 0.103 | 0.099 |
|  | 6 | Carbon tetrachloride | CCl4 | 0.000 | 310 | 5.089 | 0.850 | 0.250 | -0.307 | 0.100 | 0.097 |
|  | 7 | Carbon tetrachloride | CCl4 | 0.000 | 320 | 5.089 | 0.850 | 0.250 | -0.307 | 0.098 | 0.096 |
|  | 8 | Carbon tetrachloride | CCl4 | 0.000 | 330 | 5.089 | 0.850 | 0.250 | -0.307 | 0.096 | 0.094 |
|  | 9 | Carbon tetrachloride | CCl4 | 0.000 | 340 | 5.089 | 0.850 | 0.250 | -0.307 | 0.094 | 0.092 |
|  | 10 | Carbon tetrachloride | CCl4 | 0.000 | 350 | 5.089 | 0.850 | 0.250 | -0.307 | 0.092 | 0.090 |
|  | 11 | Carbon tetrachloride | CCl4 | 0.000 | 360 | 5.089 | 0.850 | 0.250 | -0.307 | 0.089 | 0.088 |
|  | 12 | Carbon tetrachloride | CCl4 | 0.000 | 370 | 5.089 | 0.850 | 0.250 | -0.307 | 0.087 | 0.087 |
|  | 13 | Carbon tetrachloride | CCl4 | 0.000 | 380 | 5.089 | 0.850 | 0.250 | -0.307 | 0.085 | 0.085 |
|  | 14 | Carbon tetrachloride | CCl4 | 0.000 | 390 | 5.089 | 0.850 | 0.250 | -0.307 | 0.083 | 0.083 |
|  | 15 | Carbon tetrachloride | CCl4 | 0.000 | 400 | 5.089 | 0.850 | 0.250 | -0.307 | 0.080 | 0.081 |
|  | 16 | Carbon tetrachloride | CCl4 | 0.000 | 410 | 5.089 | 0.850 | 0.250 | -0.307 | 0.078 | 0.079 |
|  | 17 | Carbon tetrachloride | CCl4 | 0.000 | 420 | 5.089 | 0.850 | 0.250 | -0.307 | 0.076 | 0.078 |
|  | 18 | Carbon tetrachloride | CCl4 | 0.000 | 430 | 5.089 | 0.850 | 0.250 | -0.307 | 0.074 | 0.076 |
|  | 19 | Carbon tetrachloride | CCl4 | 0.000 | 440 | 5.089 | 0.850 | 0.250 | -0.307 | 0.072 | 0.074 |
|  | 20 | Carbon tetrachloride | CCl4 | 0.000 | 450 | 5.089 | 0.850 | 0.250 | -0.307 | 0.070 | 0.072 |
|  | 21 | Carbon tetrachloride | CCl4 | 0.000 | 460 | 5.089 | 0.850 | 0.250 | -0.307 | 0.067 | 0.070 |
|  | 22 | Carbon tetrachloride | CCl4 | 0.000 | 470 | 5.089 | 0.850 | 0.250 | -0.307 | 0.065 | 0.069 |
|  | 23 | Trifluoromonobromo methane | CF3Br | 1.000 | 223 | 5.898 | 0.902 | 0.955 | 0.241 | 0.073 | 0.066 |
|  | 24 | Trifluoromonobromo methane | CF3Br | 1.000 | 233 | 5.898 | 0.902 | 0.955 | 0.241 | 0.069 | 0.064 |
|  | 25 | Trifluoromonobromo methane | CF3Br | 1.000 | 243 | 5.898 | 0.902 | 0.955 | 0.241 | 0.066 | 0.062 |
|  | 26 | Trifluoromonobromo methane | CF3Br | 1.000 | 253 | 5.898 | 0.902 | 0.955 | 0.241 | 0.062 | 0.060 |
|  | 27 | Trifluoromonobromo methane | CF3Br | 1.000 | 263 | 5.898 | 0.902 | 0.955 | 0.241 | 0.060 | 0.058 |
|  | 28 | Trifluoromonobromo methane | CF3Br | 1.000 | 273 | 5.898 | 0.902 | 0.955 | 0.241 | 0.056 | 0.057 |
|  | 29 | Trifluoromonobromo methane | CF3Br | 1.000 | 283 | 5.898 | 0.902 | 0.955 | 0.241 | 0.054 | 0.055 |
|  | 30 | Trifluoromonobromo methane | CF3Br | 1.000 | 293 | 5.898 | 0.902 | 0.955 | 0.241 | 0.050 | 0.053 |
|  | 31 | Trifluoromonobromo methane | CF3Br | 1.000 | 303 | 5.898 | 0.902 | 0.955 | 0.241 | 0.048 | 0.051 |
|  | 32 | Trifluoromonobromo methane | CF3Br | 1.000 | 313 | 5.898 | 0.902 | 0.955 | 0.241 | 0.045 | 0.049 |
|  | 33 | Trifluoromonobromo methane | CF3Br | 1.000 | 323 | 5.898 | 0.902 | 0.955 | 0.241 | 0.043 | 0.048 |
|  | 34 | Trifluoromonobromo methane | CF3Br | 1.000 | 333 | 5.898 | 0.902 | 0.955 | 0.241 | 0.040 | 0.046 |
|  | 35 | Trifluoromonobromo methane | CF3Br | 1.000 | 223 | 5.898 | 0.902 | 0.955 | 0.241 | 0.073 | 0.066 |
|  | 36 | Trifluoromonobromo methane | CF3Br | 1.000 | 233 | 5.898 | 0.902 | 0.955 | 0.241 | 0.069 | 0.064 |
|  | 37 | Trifluoromonobromo methane | CF3Br | 1.000 | 243 | 5.898 | 0.902 | 0.955 | 0.241 | 0.066 | 0.062 |
|  | 38 | Trifluoromonobromo methane | CF3Br | 1.000 | 253 | 5.898 | 0.902 | 0.955 | 0.241 | 0.062 | 0.060 |
|  | 39 | Trifluoromonobromo methane | CF3Br | 1.000 | 263 | 5.898 | 0.902 | 0.955 | 0.241 | 0.060 | 0.058 |
|  | 40 | Trifluoromonobromo methane | CF3Br | 1.000 | 273 | 5.898 | 0.902 | 0.955 | 0.241 | 0.056 | 0.057 |
|  | 41 | Trifluoromonobromo methane | CF3Br | 1.000 | 283 | 5.898 | 0.902 | 0.955 | 0.241 | 0.054 | 0.055 |
|  | 42 | Trifluoromonobromo methane | CF3Br | 1.000 | 293 | 5.898 | 0.902 | 0.955 | 0.241 | 0.050 | 0.053 |
|  | 43 | Trifluoromonobromo methane | CF3Br | 1.000 | 303 | 5.898 | 0.902 | 0.955 | 0.241 | 0.048 | 0.051 |
|  | 44 | Trifluoromonobromo methane | CF3Br | 1.000 | 313 | 5.898 | 0.902 | 0.955 | 0.241 | 0.045 | 0.049 |
|  | 45 | Trifluoromonobromo methane | CF3Br | 1.000 | 323 | 5.898 | 0.902 | 0.955 | 0.241 | 0.043 | 0.048 |
|  | 46 | Trifluoromonobromo methane | CF3Br | 1.000 | 333 | 5.898 | 0.902 | 0.955 | 0.241 | 0.040 | 0.046 |
|  | 47 | Bromoform | CHBr3 | 0.000 | 280 | 6.876 | 0.767 | 0.828 | -0.038 | 0.101 | 0.105 |
|  | 48 | Bromoform | CHBr3 | 0.000 | 290 | 6.876 | 0.767 | 0.828 | -0.038 | 0.100 | 0.103 |
|  | 49 | Bromoform | CHBr3 | 0.000 | 300 | 6.876 | 0.767 | 0.828 | -0.038 | 0.100 | 0.101 |
|  | 50 | Bromoform | CHBr3 | 0.000 | 310 | 6.876 | 0.767 | 0.828 | -0.038 | 0.099 | 0.099 |
|  | 51 | Bromoform | CHBr3 | 0.000 | 320 | 6.876 | 0.767 | 0.828 | -0.038 | 0.098 | 0.098 |
|  | 52 | Bromoform | CHBr3 | 0.000 | 330 | 6.876 | 0.767 | 0.828 | -0.038 | 0.098 | 0.096 |
|  | 53 | Bromoform | CHBr3 | 0.000 | 340 | 6.876 | 0.767 | 0.828 | -0.038 | 0.097 | 0.094 |
|  | 54 | Bromoform | CHBr3 | 0.000 | 350 | 6.876 | 0.767 | 0.828 | -0.038 | 0.096 | 0.092 |
|  | 55 | Bromoform | CHBr3 | 0.000 | 360 | 6.876 | 0.767 | 0.828 | -0.038 | 0.095 | 0.090 |
|  | 56 | Monofluorodichloro methane | CHFCl2 | 0.000 | 270 | 4.559 | 0.836 | 0.708 | -0.076 | 0.121 | 0.123 |
|  | 57 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 313 | 4.960 | 0.626 | 0.677 | 0.018 | 0.059 | 0.060 |
|  | 58 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 280 | 5.166 | 0.642 | 0.250 | -0.091 | 0.115 | 0.113 |
|  | 59 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 290 | 5.166 | 0.642 | 0.250 | -0.091 | 0.112 | 0.111 |
|  | 60 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 300 | 5.166 | 0.642 | 0.250 | -0.091 | 0.109 | 0.109 |
|  | 61 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 310 | 5.166 | 0.642 | 0.250 | -0.091 | 0.106 | 0.108 |
|  | 62 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 320 | 5.166 | 0.642 | 0.250 | -0.091 | 0.104 | 0.106 |
|  | 63 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 330 | 5.166 | 0.642 | 0.250 | -0.091 | 0.102 | 0.104 |
|  | 64 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 340 | 5.166 | 0.642 | 0.250 | -0.091 | 0.099 | 0.102 |
|  | 65 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 350 | 5.166 | 0.642 | 0.250 | -0.091 | 0.097 | 0.100 |
|  | 66 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 360 | 5.166 | 0.642 | 0.250 | -0.091 | 0.095 | 0.099 |
|  | 67 | Tetrachloro ethylene | CCl2CCl2 | 0.000 | 370 | 5.166 | 0.642 | 0.250 | -0.091 | 0.093 | 0.097 |
|  | 68 | Ethyl bromide | C2H5Br | 0.000 | 200 | 5.807 | 0.855 | 0.219 | 0.006 | 0.112 | 0.113 |
|  | 69 | Ethyl bromide | C2H5Br | 0.000 | 210 | 5.807 | 0.855 | 0.219 | 0.006 | 0.111 | 0.112 |
|  | 70 | Ethyl bromide | C2H5Br | 0.000 | 220 | 5.807 | 0.855 | 0.219 | 0.006 | 0.110 | 0.110 |
|  | 71 | Ethyl bromide | C2H5Br | 0.000 | 230 | 5.807 | 0.855 | 0.219 | 0.006 | 0.109 | 0.108 |
|  | 72 | Ethyl bromide | C2H5Br | 0.000 | 240 | 5.807 | 0.855 | 0.219 | 0.006 | 0.108 | 0.106 |
|  | 73 | Ethyl bromide | C2H5Br | 0.000 | 250 | 5.807 | 0.855 | 0.219 | 0.006 | 0.107 | 0.104 |
|  | 74 | Ethyl bromide | C2H5Br | 0.000 | 260 | 5.807 | 0.855 | 0.219 | 0.006 | 0.106 | 0.103 |
|  | 75 | Ethyl bromide | C2H5Br | 0.000 | 270 | 5.807 | 0.855 | 0.219 | 0.006 | 0.104 | 0.101 |
|  | 76 | Ethyl bromide | C2H5Br | 0.000 | 280 | 5.807 | 0.855 | 0.219 | 0.006 | 0.103 | 0.099 |
|  | 77 | Ethyl bromide | C2H5Br | 0.000 | 290 | 5.807 | 0.855 | 0.219 | 0.006 | 0.102 | 0.097 |
|  | 78 | Ethyl bromide | C2H5Br | 0.000 | 300 | 5.807 | 0.855 | 0.219 | 0.006 | 0.101 | 0.095 |
|  | 79 | Ethyl bromide | C2H5Br | 0.000 | 310 | 5.807 | 0.855 | 0.219 | 0.006 | 0.100 | 0.094 |
|  | 80 | Ethyl iodide | C2H5I | 0.000 | 280 | 7.116 | 0.823 | 0.222 | 0.010 | 0.090 | 0.088 |
|  | 81 | Octafluoro propane | C3F8 | 1.000 | 130 | 4.810 | 0.476 | 0.405 | -0.020 | 0.100 | 0.094 |
|  | 82 | Octafluoro propane | C3F8 | 1.000 | 140 | 4.810 | 0.476 | 0.405 | -0.020 | 0.099 | 0.093 |
|  | 83 | Octafluoro propane | C3F8 | 1.000 | 150 | 4.810 | 0.476 | 0.405 | -0.020 | 0.095 | 0.091 |
|  | 84 | Octafluoro propane | C3F8 | 1.000 | 160 | 4.810 | 0.476 | 0.405 | -0.020 | 0.091 | 0.089 |
|  | 85 | Octafluoro propane | C3F8 | 1.000 | 170 | 4.810 | 0.476 | 0.405 | -0.020 | 0.088 | 0.087 |
|  | 86 | Octafluoro propane | C3F8 | 1.000 | 180 | 4.810 | 0.476 | 0.405 | -0.020 | 0.084 | 0.085 |
|  | 87 | Octafluoro propane | C3F8 | 1.000 | 190 | 4.810 | 0.476 | 0.405 | -0.020 | 0.081 | 0.084 |
|  | 88 | Octafluoro propane | C3F8 | 1.000 | 200 | 4.810 | 0.476 | 0.405 | -0.020 | 0.077 | 0.082 |
|  | 89 | Octafluoro propane | C3F8 | 1.000 | 210 | 4.810 | 0.476 | 0.405 | -0.020 | 0.074 | 0.080 |
|  | 90 | Octafluoro propane | C3F8 | 1.000 | 130 | 4.810 | 0.476 | 0.405 | -0.020 | 0.102 | 0.094 |
|  | 91 | Octafluoro propane | C3F8 | 1.000 | 140 | 4.810 | 0.476 | 0.405 | -0.020 | 0.099 | 0.093 |
|  | 92 | Octafluoro propane | C3F8 | 1.000 | 160 | 4.810 | 0.476 | 0.405 | -0.020 | 0.092 | 0.089 |
|  | 93 | Octafluoro propane | C3F8 | 1.000 | 180 | 4.810 | 0.476 | 0.405 | -0.020 | 0.084 | 0.085 |
|  | 94 | Octafluoro propane | C3F8 | 1.000 | 200 | 4.810 | 0.476 | 0.405 | -0.020 | 0.077 | 0.082 |
|  | 95 | Octafluoro propane | C3F8 | 1.000 | 220 | 4.810 | 0.476 | 0.405 | -0.020 | 0.071 | 0.078 |
|  | 96 | n-Propyl bromide | C3H7Br | 0.000 | 230 | 5.827 | 0.761 | 0.175 | 0.055 | 0.112 | 0.111 |
|  | 97 | n-Propyl bromide | C3H7Br | 0.000 | 240 | 5.827 | 0.761 | 0.175 | 0.055 | 0.110 | 0.109 |
|  | 98 | n-Propyl bromide | C3H7Br | 0.000 | 250 | 5.827 | 0.761 | 0.175 | 0.055 | 0.108 | 0.108 |
|  | 99 | n-Propyl bromide | C3H7Br | 0.000 | 260 | 5.827 | 0.761 | 0.175 | 0.055 | 0.106 | 0.106 |
|  | 100 | n-Propyl bromide | C3H7Br | 0.000 | 270 | 5.827 | 0.761 | 0.175 | 0.055 | 0.105 | 0.104 |
|  | 101 | n-Propyl bromide | C3H7Br | 0.000 | 280 | 5.827 | 0.761 | 0.175 | 0.055 | 0.103 | 0.102 |
|  | 102 | n-Propyl bromide | C3H7Br | 0.000 | 290 | 5.827 | 0.761 | 0.175 | 0.055 | 0.101 | 0.100 |
|  | 103 | n-Propyl bromide | C3H7Br | 0.000 | 300 | 5.827 | 0.761 | 0.175 | 0.055 | 0.099 | 0.099 |
|  | 104 | n-Propyl bromide | C3H7Br | 0.000 | 310 | 5.827 | 0.761 | 0.175 | 0.055 | 0.098 | 0.097 |
|  | 105 | n-Propyl bromide | C3H7Br | 0.000 | 320 | 5.827 | 0.761 | 0.175 | 0.055 | 0.096 | 0.095 |
|  | 106 | n-Propyl bromide | C3H7Br | 0.000 | 330 | 5.827 | 0.761 | 0.175 | 0.055 | 0.094 | 0.093 |
|  | 107 | n-Propyl iodide | C3H7I | 0.000 | 280 | 7.122 | 0.753 | 0.175 | -0.024 | 0.091 | 0.089 |
|  | 108 | n-Propyl iodide | C3H7I | 0.000 | 290 | 7.122 | 0.753 | 0.175 | -0.024 | 0.089 | 0.088 |
|  | 109 | n-Propyl iodide | C3H7I | 0.000 | 300 | 7.122 | 0.753 | 0.175 | -0.024 | 0.087 | 0.086 |
|  | 110 | n-Propyl iodide | C3H7I | 0.000 | 310 | 7.122 | 0.753 | 0.175 | -0.024 | 0.085 | 0.084 |
|  | 111 | n-Propyl iodide | C3H7I | 0.000 | 320 | 7.122 | 0.753 | 0.175 | -0.024 | 0.083 | 0.082 |
|  | 112 | n-Propyl iodide | C3H7I | 0.000 | 330 | 7.122 | 0.753 | 0.175 | -0.024 | 0.082 | 0.080 |
|  | 113 | n-Propyl iodide | C3H7I | 0.000 | 340 | 7.122 | 0.753 | 0.175 | -0.024 | 0.080 | 0.079 |
|  | 114 | n-Propyl iodide | C3H7I | 0.000 | 350 | 7.122 | 0.753 | 0.175 | -0.024 | 0.078 | 0.077 |
|  | 115 | butyl bromide | C4H9Br | 0.000 | 210 | 5.848 | 0.637 | 0.143 | 0.036 | 0.119 | 0.119 |
|  | 116 | butyl bromide | C4H9Br | 0.000 | 220 | 5.848 | 0.637 | 0.143 | 0.036 | 0.117 | 0.117 |
|  | 117 | butyl bromide | C4H9Br | 0.000 | 230 | 5.848 | 0.637 | 0.143 | 0.036 | 0.115 | 0.115 |
|  | 118 | butyl bromide | C4H9Br | 0.000 | 240 | 5.848 | 0.637 | 0.143 | 0.036 | 0.113 | 0.113 |
|  | 119 | butyl bromide | C4H9Br | 0.000 | 250 | 5.848 | 0.637 | 0.143 | 0.036 | 0.111 | 0.111 |
|  | 120 | butyl bromide | C4H9Br | 0.000 | 260 | 5.848 | 0.637 | 0.143 | 0.036 | 0.110 | 0.110 |
|  | 121 | butyl bromide | C4H9Br | 0.000 | 270 | 5.848 | 0.637 | 0.143 | 0.036 | 0.108 | 0.108 |
|  | 122 | butyl bromide | C4H9Br | 0.000 | 280 | 5.848 | 0.637 | 0.143 | 0.036 | 0.106 | 0.106 |
|  | 123 | butyl bromide | C4H9Br | 0.000 | 290 | 5.848 | 0.637 | 0.143 | 0.036 | 0.104 | 0.104 |
|  | 124 | butyl bromide | C4H9Br | 0.000 | 300 | 5.848 | 0.637 | 0.143 | 0.036 | 0.102 | 0.102 |
|  | 125 | butyl bromide | C4H9Br | 0.000 | 310 | 5.848 | 0.637 | 0.143 | 0.036 | 0.100 | 0.101 |
|  | 126 | butyl bromide | C4H9Br | 0.000 | 320 | 5.848 | 0.637 | 0.143 | 0.036 | 0.098 | 0.099 |
|  | 127 | butyl bromide | C4H9Br | 0.000 | 330 | 5.848 | 0.637 | 0.143 | 0.036 | 0.096 | 0.097 |
|  | 128 | butyl bromide | C4H9Br | 0.000 | 340 | 5.848 | 0.637 | 0.143 | 0.036 | 0.094 | 0.095 |
|  | 129 | butyl bromide | C4H9Br | 0.000 | 350 | 5.848 | 0.637 | 0.143 | 0.036 | 0.093 | 0.093 |
|  | 130 | butyl bromide | C4H9Br | 0.000 | 360 | 5.848 | 0.637 | 0.143 | 0.036 | 0.091 | 0.092 |
|  | 131 | isobutyl bromide | C4H9Br | 0.000 | 280 | 5.852 | 0.782 | 0.167 | 0.020 | 0.097 | 0.101 |
|  | 132 | isobutyl bromide | C4H9Br | 0.000 | 290 | 5.852 | 0.782 | 0.167 | 0.020 | 0.095 | 0.099 |
|  | 133 | isobutyl bromide | C4H9Br | 0.000 | 300 | 5.852 | 0.782 | 0.167 | 0.020 | 0.093 | 0.097 |
|  | 134 | isobutyl bromide | C4H9Br | 0.000 | 310 | 5.852 | 0.782 | 0.167 | 0.020 | 0.092 | 0.095 |
|  | 135 | isobutyl bromide | C4H9Br | 0.000 | 320 | 5.852 | 0.782 | 0.167 | 0.020 | 0.090 | 0.093 |
|  | 136 | isobutyl bromide | C4H9Br | 0.000 | 330 | 5.852 | 0.782 | 0.167 | 0.020 | 0.088 | 0.092 |
|  | 137 | isobutyl bromide | C4H9Br | 0.000 | 340 | 5.852 | 0.782 | 0.167 | 0.020 | 0.087 | 0.090 |
|  | 138 | isobutyl bromide | C4H9Br | 0.000 | 350 | 5.852 | 0.782 | 0.167 | 0.020 | 0.085 | 0.088 |
|  | 139 | butyl iodide | C4H9I | 0.000 | 280 | 7.128 | 0.634 | 0.144 | -0.066 | 0.092 | 0.093 |
|  | 140 | butyl iodide | C4H9I | 0.000 | 290 | 7.128 | 0.634 | 0.144 | -0.066 | 0.091 | 0.091 |
|  | 141 | butyl iodide | C4H9I | 0.000 | 300 | 7.128 | 0.634 | 0.144 | -0.066 | 0.089 | 0.089 |
|  | 142 | butyl iodide | C4H9I | 0.000 | 310 | 7.128 | 0.634 | 0.144 | -0.066 | 0.087 | 0.087 |
|  | 143 | butyl iodide | C4H9I | 0.000 | 320 | 7.128 | 0.634 | 0.144 | -0.066 | 0.086 | 0.086 |
|  | 144 | butyl iodide | C4H9I | 0.000 | 330 | 7.128 | 0.634 | 0.144 | -0.066 | 0.084 | 0.084 |
|  | 145 | butyl iodide | C4H9I | 0.000 | 340 | 7.128 | 0.634 | 0.144 | -0.066 | 0.082 | 0.082 |
|  | 146 | butyl iodide | C4H9I | 0.000 | 350 | 7.128 | 0.634 | 0.144 | -0.066 | 0.081 | 0.080 |
|  | 147 | butyl iodide | C4H9I | 0.000 | 360 | 7.128 | 0.634 | 0.144 | -0.066 | 0.079 | 0.078 |
|  | 148 | butyl iodide | C4H9I | 0.000 | 370 | 7.128 | 0.634 | 0.144 | -0.066 | 0.077 | 0.077 |
|  | 149 | butyl iodide | C4H9I | 0.000 | 380 | 7.128 | 0.634 | 0.144 | -0.066 | 0.076 | 0.075 |
|  | 150 | isobutyl iodide | C4H9I | 0.000 | 280 | 7.129 | 0.780 | 0.17 | -0.071 | 0.086 | 0.088 |
|  | 151 | isobutyl iodide | C4H9I | 0.000 | 320 | 7.129 | 0.780 | 0.17 | -0.071 | 0.080 | 0.080 |
|  | 152 | isobutyl iodide | C4H9I | 0.000 | 350 | 7.129 | 0.780 | 0.17 | -0.071 | 0.076 | 0.075 |
|  | 153 | n-amyl bromide | C5H11Br | 0.000 | 220 | 5.868 | 0.538 | 0.118 | 0.017 | 0.118 | 0.120 |
|  | 154 | n-amyl bromide | C5H11Br | 0.000 | 230 | 5.868 | 0.538 | 0.118 | 0.017 | 0.116 | 0.118 |
|  | 155 | n-amyl bromide | C5H11Br | 0.000 | 240 | 5.868 | 0.538 | 0.118 | 0.017 | 0.114 | 0.116 |
|  | 156 | n-amyl bromide | C5H11Br | 0.000 | 250 | 5.868 | 0.538 | 0.118 | 0.017 | 0.113 | 0.114 |
|  | 157 | n-amyl bromide | C5H11Br | 0.000 | 260 | 5.868 | 0.538 | 0.118 | 0.017 | 0.111 | 0.112 |
|  | 158 | n-amyl bromide | C5H11Br | 0.000 | 270 | 5.868 | 0.538 | 0.118 | 0.017 | 0.110 | 0.111 |
|  | 159 | n-amyl bromide | C5H11Br | 0.000 | 280 | 5.868 | 0.538 | 0.118 | 0.017 | 0.108 | 0.109 |
|  | 160 | n-amyl bromide | C5H11Br | 0.000 | 290 | 5.868 | 0.538 | 0.118 | 0.017 | 0.106 | 0.107 |
|  | 161 | n-amyl bromide | C5H11Br | 0.000 | 300 | 5.868 | 0.538 | 0.118 | 0.017 | 0.105 | 0.105 |
|  | 162 | n-amyl bromide | C5H11Br | 0.000 | 310 | 5.868 | 0.538 | 0.118 | 0.017 | 0.103 | 0.104 |
|  | 163 | n-amyl bromide | C5H11Br | 0.000 | 320 | 5.868 | 0.538 | 0.118 | 0.017 | 0.101 | 0.102 |
|  | 164 | n-amyl bromide | C5H11Br | 0.000 | 330 | 5.868 | 0.538 | 0.118 | 0.017 | 0.100 | 0.100 |
|  | 165 | n-amyl bromide | C5H11Br | 0.000 | 340 | 5.868 | 0.538 | 0.118 | 0.017 | 0.098 | 0.098 |
|  | 166 | n-amyl bromide | C5H11Br | 0.000 | 350 | 5.868 | 0.538 | 0.118 | 0.017 | 0.096 | 0.096 |
|  | 167 | n-amyl bromide | C5H11Br | 0.000 | 360 | 5.868 | 0.538 | 0.118 | 0.017 | 0.095 | 0.095 |
|  | 168 | n-amyl bromide | C5H11Br | 0.000 | 370 | 5.868 | 0.538 | 0.118 | 0.017 | 0.093 | 0.093 |
|  | 169 | n-amyl bromide | C5H11Br | 0.000 | 380 | 5.868 | 0.538 | 0.118 | 0.017 | 0.091 | 0.091 |
|  | 170 | n-amyl chloride | C5H11Cl | 0.000 | 270 | 4.268 | 0.539 | 0.113 | -0.025 | 0.126 | 0.125 |
|  | 171 | n-amyl chloride | C5H11Cl | 0.000 | 280 | 4.268 | 0.539 | 0.113 | -0.025 | 0.124 | 0.123 |
|  | 172 | n-amyl chloride | C5H11Cl | 0.000 | 290 | 4.268 | 0.539 | 0.113 | -0.025 | 0.122 | 0.122 |
|  | 173 | n-amyl chloride | C5H11Cl | 0.000 | 300 | 4.268 | 0.539 | 0.113 | -0.025 | 0.119 | 0.120 |
|  | 174 | n-amyl chloride | C5H11Cl | 0.000 | 310 | 4.268 | 0.539 | 0.113 | -0.025 | 0.117 | 0.118 |
|  | 175 | n-amyl chloride | C5H11Cl | 0.000 | 320 | 4.268 | 0.539 | 0.113 | -0.025 | 0.115 | 0.116 |
|  | 176 | n-amyl chloride | C5H11Cl | 0.000 | 330 | 4.268 | 0.539 | 0.113 | -0.025 | 0.113 | 0.114 |
|  | 177 | n-amyl chloride | C5H11Cl | 0.000 | 340 | 4.268 | 0.539 | 0.113 | -0.025 | 0.111 | 0.113 |
|  | 178 | n-amyl chloride | C5H11Cl | 0.000 | 350 | 4.268 | 0.539 | 0.113 | -0.025 | 0.109 | 0.111 |
|  | 179 | n-amyl iodide | C5H11I | 0.000 | 280 | 7.133 | 0.537 | 0.118 | 0.002 | 0.095 | 0.097 |
|  | 180 | n-amyl iodide | C5H11I | 0.000 | 290 | 7.133 | 0.537 | 0.118 | 0.002 | 0.093 | 0.095 |
|  | 181 | n-amyl iodide | C5H11I | 0.000 | 300 | 7.133 | 0.537 | 0.118 | 0.002 | 0.092 | 0.093 |
|  | 182 | n-amyl iodide | C5H11I | 0.000 | 310 | 7.133 | 0.537 | 0.118 | 0.002 | 0.090 | 0.091 |
|  | 183 | n-amyl iodide | C5H11I | 0.000 | 320 | 7.133 | 0.537 | 0.118 | 0.002 | 0.088 | 0.090 |
|  | 184 | n-amyl iodide | C5H11I | 0.000 | 330 | 7.133 | 0.537 | 0.118 | 0.002 | 0.087 | 0.088 |
|  | 185 | n-amyl iodide | C5H11I | 0.000 | 340 | 7.133 | 0.537 | 0.118 | 0.002 | 0.085 | 0.086 |
|  | 186 | n-amyl iodide | C5H11I | 0.000 | 350 | 7.133 | 0.537 | 0.118 | 0.002 | 0.084 | 0.084 |
|  | 187 | n-amyl iodide | C5H11I | 0.000 | 360 | 7.133 | 0.537 | 0.118 | 0.002 | 0.082 | 0.082 |
|  | 188 | n-amyl iodide | C5H11I | 0.000 | 370 | 7.133 | 0.537 | 0.118 | 0.002 | 0.081 | 0.081 |
|  | 189 | n-amyl iodide | C5H11I | 0.000 | 380 | 7.133 | 0.537 | 0.118 | 0.002 | 0.079 | 0.079 |
|  | 190 | n-amyl iodide | C5H11I | 0.000 | 390 | 7.133 | 0.537 | 0.118 | 0.002 | 0.078 | 0.077 |
|  | 191 | n-amyl iodide | C5H11I | 0.000 | 400 | 7.133 | 0.537 | 0.118 | 0.002 | 0.076 | 0.075 |
|  | 192 | n-amyl iodide | C5H11I | 0.000 | 410 | 7.133 | 0.537 | 0.118 | 0.002 | 0.075 | 0.074 |
|  | 193 | isoamyl iodide | C5H11I | 0.000 | 280 | 7.134 | 0.640 | 0.123 | -0.013 | 0.088 | 0.093 |
|  | 194 | isoamyl iodide | C5H11I | 0.000 | 330 | 7.134 | 0.640 | 0.123 | -0.013 | 0.081 | 0.084 |
|  | 195 | isoamyl iodide | C5H11I | 0.000 | 360 | 7.134 | 0.640 | 0.123 | -0.013 | 0.077 | 0.078 |
|  | 196 | isoamyl iodide | C5H11I | 0.000 | 390 | 7.134 | 0.640 | 0.123 | -0.013 | 0.074 | 0.073 |
|  | 197 | n-bromo hexane | C6H13Br | 0.000 | 240 | 5.888 | 0.463 | 0.101 | 0.074 | 0.117 | 0.119 |
|  | 198 | n-bromo hexane | C6H13Br | 0.000 | 250 | 5.888 | 0.463 | 0.101 | 0.074 | 0.115 | 0.117 |
|  | 199 | n-bromo hexane | C6H13Br | 0.000 | 260 | 5.888 | 0.463 | 0.101 | 0.074 | 0.114 | 0.116 |
|  | 200 | n-bromo hexane | C6H13Br | 0.000 | 270 | 5.888 | 0.463 | 0.101 | 0.074 | 0.113 | 0.114 |
|  | 201 | n-bromo hexane | C6H13Br | 0.000 | 280 | 5.888 | 0.463 | 0.101 | 0.074 | 0.111 | 0.112 |
|  | 202 | n-bromo hexane | C6H13Br | 0.000 | 290 | 5.888 | 0.463 | 0.101 | 0.074 | 0.110 | 0.110 |
|  | 203 | n-bromo hexane | C6H13Br | 0.000 | 300 | 5.888 | 0.463 | 0.101 | 0.074 | 0.108 | 0.108 |
|  | 204 | n-bromo hexane | C6H13Br | 0.000 | 310 | 5.888 | 0.463 | 0.101 | 0.074 | 0.106 | 0.107 |
|  | 205 | n-bromo hexane | C6H13Br | 0.000 | 320 | 5.888 | 0.463 | 0.101 | 0.074 | 0.104 | 0.105 |
|  | 206 | n-bromo hexane | C6H13Br | 0.000 | 330 | 5.888 | 0.463 | 0.101 | 0.074 | 0.102 | 0.103 |
|  | 207 | n-bromo hexane | C6H13Br | 0.000 | 340 | 5.888 | 0.463 | 0.101 | 0.074 | 0.101 | 0.101 |
|  | 208 | n-bromo hexane | C6H13Br | 0.000 | 350 | 5.888 | 0.463 | 0.101 | 0.074 | 0.099 | 0.099 |
|  | 209 | n-bromo hexane | C6H13Br | 0.000 | 360 | 5.888 | 0.463 | 0.101 | 0.074 | 0.098 | 0.098 |
|  | 210 | n-bromo hexane | C6H13Br | 0.000 | 370 | 5.888 | 0.463 | 0.101 | 0.074 | 0.096 | 0.096 |
|  | 211 | n-bromo hexane | C6H13Br | 0.000 | 380 | 5.888 | 0.463 | 0.101 | 0.074 | 0.095 | 0.094 |
|  | 212 | n-bromo hexane | C6H13Br | 0.000 | 390 | 5.888 | 0.463 | 0.101 | 0.074 | 0.093 | 0.092 |
|  | 213 | n-bromo hexane | C6H13Br | 0.000 | 400 | 5.888 | 0.463 | 0.101 | 0.074 | 0.091 | 0.090 |
|  | 214 | n-hexyl iodide | C6H13I | 0.000 | 280 | 7.139 | 0.462 | 0.101 | 0.035 | 0.097 | 0.100 |
|  | 215 | n-hexyl iodide | C6H13I | 0.000 | 300 | 7.139 | 0.462 | 0.101 | 0.035 | 0.094 | 0.096 |
|  | 216 | n-hexyl iodide | C6H13I | 0.000 | 320 | 7.139 | 0.462 | 0.101 | 0.035 | 0.091 | 0.093 |
|  | 217 | n-hexyl iodide | C6H13I | 0.000 | 340 | 7.139 | 0.462 | 0.101 | 0.035 | 0.088 | 0.089 |
|  | 218 | n-hexyl iodide | C6H13I | 0.000 | 360 | 7.139 | 0.462 | 0.101 | 0.035 | 0.085 | 0.085 |
|  | 219 | n-hexyl iodide | C6H13I | 0.000 | 380 | 7.139 | 0.462 | 0.101 | 0.035 | 0.082 | 0.082 |
|  | 220 | n-hexyl iodide | C6H13I | 0.000 | 400 | 7.139 | 0.462 | 0.101 | 0.035 | 0.080 | 0.078 |
|  | 221 | n-hexyl iodide | C6H13I | 0.000 | 410 | 7.139 | 0.462 | 0.101 | 0.035 | 0.078 | 0.076 |
|  | 222 | n-perfluoro heptane | C7F16 | 1.000 | 223 | 5.551 | 0.233 | 0.215 | -0.072 | 0.071 | 0.076 |
|  | 223 | n-perfluoro heptane | C7F16 | 1.000 | 233 | 5.551 | 0.233 | 0.215 | -0.072 | 0.070 | 0.074 |
|  | 224 | n-perfluoro heptane | C7F16 | 1.000 | 253 | 5.551 | 0.233 | 0.215 | -0.072 | 0.067 | 0.070 |
|  | 225 | n-perfluoro heptane | C7F16 | 1.000 | 273 | 5.551 | 0.233 | 0.215 | -0.072 | 0.064 | 0.067 |
|  | 226 | n-perfluoro heptane | C7F16 | 1.000 | 293 | 5.551 | 0.233 | 0.215 | -0.072 | 0.061 | 0.063 |
|  | 227 | n-perfluoro heptane | C7F16 | 1.000 | 313 | 5.551 | 0.233 | 0.215 | -0.072 | 0.058 | 0.059 |
|  | 228 | n-perfluoro heptane | C7F16 | 1.000 | 333 | 5.551 | 0.233 | 0.215 | -0.072 | 0.054 | 0.056 |
|  | 229 | n-perfluoro heptane | C7F16 | 1.000 | 353 | 5.551 | 0.233 | 0.215 | -0.072 | 0.051 | 0.052 |
|  | 230 | 1-bromo heptane | C7H15Br | 0.000 | 260 | 5.907 | 0.404 | 0.089 | 0.185 | 0.114 | 0.119 |
|  | 231 | 1-bromo heptane | C7H15Br | 0.000 | 280 | 5.907 | 0.404 | 0.089 | 0.185 | 0.112 | 0.115 |
|  | 232 | 1-bromo heptane | C7H15Br | 0.000 | 300 | 5.907 | 0.404 | 0.089 | 0.185 | 0.109 | 0.112 |
|  | 233 | 1-bromo heptane | C7H15Br | 0.000 | 320 | 5.907 | 0.404 | 0.089 | 0.185 | 0.106 | 0.108 |
|  | 234 | 1-bromo heptane | C7H15Br | 0.000 | 340 | 5.907 | 0.404 | 0.089 | 0.185 | 0.103 | 0.105 |
|  | 235 | 1-bromo heptane | C7H15Br | 0.000 | 360 | 5.907 | 0.404 | 0.089 | 0.185 | 0.101 | 0.101 |
|  | 236 | 1-bromo heptane | C7H15Br | 0.000 | 380 | 5.907 | 0.404 | 0.089 | 0.185 | 0.098 | 0.097 |
|  | 237 | 1-bromo heptane | C7H15Br | 0.000 | 390 | 5.907 | 0.404 | 0.089 | 0.185 | 0.097 | 0.096 |
|  | 238 | 1-chloro heptane | C7H15Cl | 0.000 | 280 | 4.447 | 0.405 | 0.085 | 0.085 | 0.127 | 0.128 |
|  | 239 | 1-chloro heptane | C7H15Cl | 0.000 | 300 | 4.447 | 0.405 | 0.085 | 0.085 | 0.123 | 0.124 |
|  | 240 | 1-chloro heptane | C7H15Cl | 0.000 | 320 | 4.447 | 0.405 | 0.085 | 0.085 | 0.120 | 0.121 |
|  | 241 | 1-chloro heptane | C7H15Cl | 0.000 | 340 | 4.447 | 0.405 | 0.085 | 0.085 | 0.116 | 0.117 |
|  | 242 | 1-chloro heptane | C7H15Cl | 0.000 | 360 | 4.447 | 0.405 | 0.085 | 0.085 | 0.113 | 0.113 |
|  | 243 | 1-chloro heptane | C7H15Cl | 0.000 | 380 | 4.447 | 0.405 | 0.085 | 0.085 | 0.110 | 0.110 |
|  | 244 | 1-chloro heptane | C7H15Cl | 0.000 | 400 | 4.447 | 0.405 | 0.085 | 0.085 | 0.106 | 0.106 |
|  | 245 | 1-chloro heptane | C7H15Cl | 0.000 | 410 | 4.447 | 0.405 | 0.085 | 0.085 | 0.105 | 0.104 |
|  | 246 | decyl bromide | C10H21Br | 0.000 | 293 | 5.962 | 0.291 | 0.065 | 0.291 | 0.126 | 0.118 |
|  | 247 | decyl bromide | C10H21Br | 0.000 | 310 | 5.962 | 0.291 | 0.065 | 0.291 | 0.114 | 0.115 |
|  | 248 | decyl bromide | C10H21Br | 0.000 | 330 | 5.962 | 0.291 | 0.065 | 0.291 | 0.112 | 0.111 |
|  | 249 | decyl bromide | C10H21Br | 0.000 | 350 | 5.962 | 0.291 | 0.065 | 0.291 | 0.110 | 0.107 |
|  | 250 | decyl bromide | C10H21Br | 0.000 | 370 | 5.962 | 0.291 | 0.065 | 0.291 | 0.107 | 0.104 |
|  | 251 | decyl bromide | C10H21Br | 0.000 | 390 | 5.962 | 0.291 | 0.065 | 0.291 | 0.105 | 0.100 |
|  | 252 | decyl bromide | C10H21Br | 0.000 | 410 | 5.962 | 0.291 | 0.065 | 0.291 | 0.102 | 0.097 |
|  | 253 | isodecyl bromide | C10H21Br | 0.000 | 420 | 5.962 | 0.291 | 0.065 | 0.291 | 0.101 | 0.095 |
|  | 254 | isodecyl bromide | C10H21Br | 0.000 | 310 | 5.962 | 0.291 | 0.064 | 0.271 | 0.116 | 0.114 |
|  | 255 | isodecyl bromide | C10H21Br | 0.000 | 320 | 5.962 | 0.291 | 0.064 | 0.271 | 0.112 | 0.113 |
|  | 256 | isodecyl bromide | C10H21Br | 0.000 | 330 | 5.962 | 0.291 | 0.064 | 0.271 | 0.108 | 0.111 |
|  | 257 | isodecyl bromide | C10H21Br | 0.000 | 340 | 5.962 | 0.291 | 0.064 | 0.271 | 0.104 | 0.109 |
|  | 258 | isodecyl chloride | C10H21Cl | 0.000 | 320 | 4.667 | 0.291 | 0.064 | 0.074 | 0.127 | 0.122 |
|  | 259 | isodecyl chloride | C10H21Cl | 0.000 | 330 | 4.667 | 0.291 | 0.064 | 0.074 | 0.123 | 0.121 |
|  | 260 | isodecyl chloride | C10H21Cl | 0.000 | 340 | 4.667 | 0.291 | 0.064 | 0.074 | 0.120 | 0.119 |
|  | 261 | n-perfluoro octane | C8F18 | 1.000 | 273 | 5.674 | 0.206 | 0.193 | -0.142 | 0.067 | 0.065 |
|  | 262 | n-perfluoro octane | C8F18 | 1.000 | 283 | 5.674 | 0.206 | 0.193 | -0.142 | 0.066 | 0.063 |
|  | 263 | n-perfluoro octane | C8F18 | 1.000 | 293 | 5.674 | 0.206 | 0.193 | -0.142 | 0.063 | 0.062 |
|  | 264 | n-perfluoro octane | C8F18 | 1.000 | 313 | 5.674 | 0.206 | 0.193 | -0.142 | 0.060 | 0.058 |
|  | 265 | n-perfluoro octane | C8F18 | 1.000 | 333 | 5.674 | 0.206 | 0.193 | -0.142 | 0.057 | 0.054 |
|  | 266 | n-perfluoro octane | C8F18 | 1.000 | 353 | 5.674 | 0.206 | 0.193 | -0.142 | 0.055 | 0.051 |
|  | 267 | n-perfluoro octane | C8F18 | 1.000 | 373 | 5.674 | 0.206 | 0.193 | -0.142 | 0.052 | 0.047 |
|  | 268 | n-octyl chloride | C8H17Cl | 0.000 | 340 | 4.526 | 0.359 | 0.074 | 0.212 | 0.122 | 0.119 |
|  | 269 | n-octyl iodide | C8H17I | 0.000 | 280 | 7.150 | 0.358 | 0.085 | 0.247 | 0.102 | 0.106 |
|  | 270 | n-octyl iodide | C8H17I | 0.000 | 300 | 7.150 | 0.358 | 0.085 | 0.247 | 0.099 | 0.102 |
|  | 271 | n-octyl iodide | C8H17I | 0.000 | 320 | 7.150 | 0.358 | 0.085 | 0.247 | 0.097 | 0.099 |
|  | 272 | n-octyl iodide | C8H17I | 0.000 | 340 | 7.150 | 0.358 | 0.085 | 0.247 | 0.094 | 0.095 |
|  | 273 | n-octyl iodide | C8H17I | 0.000 | 360 | 7.150 | 0.358 | 0.085 | 0.247 | 0.091 | 0.092 |
|  | 274 | n-octyl iodide | C8H17I | 0.000 | 380 | 7.150 | 0.358 | 0.085 | 0.247 | 0.089 | 0.088 |
|  | 275 | n-octyl iodide | C8H17I | 0.000 | 400 | 7.150 | 0.358 | 0.085 | 0.247 | 0.086 | 0.085 |
|  | 276 | n-octyl iodide | C8H17I | 0.000 | 420 | 7.150 | 0.358 | 0.085 | 0.247 | 0.083 | 0.081 |
|  | 277 | n-octyl iodide | C8H17I | 0.000 | 440 | 7.150 | 0.358 | 0.085 | 0.247 | 0.081 | 0.077 |
|  | 278 | n-octyl iodide | C8H17I | 0.000 | 450 | 7.150 | 0.358 | 0.085 | 0.247 | 0.079 | 0.076 |
|  | 279 | n-nonyl bromide | C9H19Br | 0.000 | 280 | 5.944 | 0.322 | 0.073 | 0.380 | 0.115 | 0.120 |
|  | 280 | n-nonyl bromide | C9H19Br | 0.000 | 300 | 5.944 | 0.322 | 0.073 | 0.380 | 0.113 | 0.117 |
|  | 281 | n-nonyl bromide | C9H19Br | 0.000 | 320 | 5.944 | 0.322 | 0.073 | 0.380 | 0.110 | 0.113 |
|  | 282 | n-nonyl bromide | C9H19Br | 0.000 | 340 | 5.944 | 0.322 | 0.073 | 0.380 | 0.108 | 0.109 |
|  | 283 | n-nonyl bromide | C9H19Br | 0.000 | 360 | 5.944 | 0.322 | 0.073 | 0.380 | 0.105 | 0.106 |
|  | 284 | n-nonyl bromide | C9H19Br | 0.000 | 380 | 5.944 | 0.322 | 0.073 | 0.380 | 0.103 | 0.102 |
|  | 285 | n-nonyl bromide | C9H19Br | 0.000 | 400 | 5.944 | 0.322 | 0.073 | 0.380 | 0.100 | 0.099 |
|  | 286 | n-nonyl bromide | C9H19Br | 0.000 | 420 | 5.944 | 0.322 | 0.073 | 0.380 | 0.098 | 0.095 |
|  | 287 | n-nonyl bromide | C9H19Br | 0.000 | 440 | 5.944 | 0.322 | 0.073 | 0.380 | 0.095 | 0.092 |
|  | 288 | n-nonyl chloride | C9H19Cl | 0.000 | 280 | 4.599 | 0.322 | 0.067 | 0.243 | 0.130 | 0.131 |
|  | 289 | n-nonyl chloride | C9H19Cl | 0.000 | 300 | 4.599 | 0.322 | 0.067 | 0.243 | 0.127 | 0.128 |
|  | 290 | n-nonyl chloride | C9H19Cl | 0.000 | 320 | 4.599 | 0.322 | 0.067 | 0.243 | 0.124 | 0.124 |
|  | 291 | n-nonyl chloride | C9H19Cl | 0.000 | 340 | 4.599 | 0.322 | 0.067 | 0.243 | 0.120 | 0.120 |
|  | 292 | n-nonyl chloride | C9H19Cl | 0.000 | 360 | 4.599 | 0.322 | 0.067 | 0.243 | 0.117 | 0.117 |
|  | 293 | n-nonyl chloride | C9H19Cl | 0.000 | 380 | 4.599 | 0.322 | 0.067 | 0.243 | 0.114 | 0.113 |
|  | 294 | n-nonyl chloride | C9H19Cl | 0.000 | 400 | 4.599 | 0.322 | 0.067 | 0.243 | 0.110 | 0.110 |
|  | 295 | n-nonyl chloride | C9H19Cl | 0.000 | 420 | 4.599 | 0.322 | 0.067 | 0.243 | 0.107 | 0.106 |
|  | 296 | n-nonyl chloride | C9H19Cl | 0.000 | 440 | 4.599 | 0.322 | 0.067 | 0.243 | 0.103 | 0.102 |
|  | 297 | n-nonyl chloride | C9H19Cl | 0.000 | 450 | 4.599 | 0.322 | 0.067 | 0.243 | 0.102 | 0.101 |
|  | 298 | n-nonyl iodide | C9H19I | 0.000 | 280 | 7.155 | 0.321 | 0.081 | 0.235 | 0.105 | 0.107 |
|  | 299 | n-nonyl iodide | C9H19I | 0.000 | 300 | 7.155 | 0.321 | 0.081 | 0.235 | 0.102 | 0.104 |
|  | 300 | n-nonyl iodide | C9H19I | 0.000 | 320 | 7.155 | 0.321 | 0.081 | 0.235 | 0.099 | 0.100 |
|  | 301 | n-nonyl iodide | C9H19I | 0.000 | 340 | 7.155 | 0.321 | 0.081 | 0.235 | 0.097 | 0.096 |
|  | 302 | n-nonyl iodide | C9H19I | 0.000 | 360 | 7.155 | 0.321 | 0.081 | 0.235 | 0.094 | 0.093 |
|  | 303 | n-nonyl iodide | C9H19I | 0.000 | 380 | 7.155 | 0.321 | 0.081 | 0.235 | 0.091 | 0.089 |
|  | 304 | n-nonyl iodide | C9H19I | 0.000 | 400 | 7.155 | 0.321 | 0.081 | 0.235 | 0.089 | 0.086 |
|  | 305 | n-nonyl iodide | C9H19I | 0.000 | 420 | 7.155 | 0.321 | 0.081 | 0.235 | 0.086 | 0.082 |
|  | 306 | n-nonyl iodide | C9H19I | 0.000 | 440 | 7.155 | 0.321 | 0.081 | 0.235 | 0.083 | 0.079 |
|  | 307 | n-nonyl iodide | C9H19I | 0.000 | 450 | 7.155 | 0.321 | 0.081 | 0.235 | 0.082 | 0.077 |
| **Prediction set** | 308 | Monofluorodichloro methane | CHFCl2 | 0.000 | 250 | 5.089 | 0.85 | 0.25 | -0.307 | 0.114 | 0.108 |
|  | 309 | Monofluorodichloro methane | CHFCl2 | 0.000 | 270 | 4.559 | 0.836 | 0.708 | -0.076 | 0.121 | 0.123 |
|  | 310 | Monofluorodichloro methane | CHFCl2 | 0.000 | 280 | 4.559 | 0.836 | 0.708 | -0.076 | 0.119 | 0.121 |
|  | 311 | Monofluorodichloro methane | CHFCl2 | 0.000 | 290 | 4.559 | 0.836 | 0.708 | -0.076 | 0.118 | 0.119 |
|  | 312 | Monofluorodichloro methane | CHFCl2 | 0.000 | 300 | 4.559 | 0.836 | 0.708 | -0.076 | 0.116 | 0.117 |
|  | 313 | Monofluorodichloro methane | CHFCl2 | 0.000 | 310 | 4.559 | 0.836 | 0.708 | -0.076 | 0.114 | 0.115 |
|  | 314 | Monofluorodichloro methane | CHFCl2 | 0.000 | 320 | 4.559 | 0.836 | 0.708 | -0.076 | 0.112 | 0.114 |
|  | 315 | Monofluorodichloro methane | CHFCl2 | 0.000 | 330 | 4.559 | 0.836 | 0.708 | -0.076 | 0.111 | 0.112 |
|  | 316 | Monofluorodichloro methane | CHFCl2 | 0.000 | 340 | 4.559 | 0.836 | 0.708 | -0.076 | 0.109 | 0.110 |
|  | 317 | Monofluorodichloro methane | CHFCl2 | 0.000 | 280 | 4.559 | 0.836 | 0.708 | -0.076 | 0.119 | 0.121 |
|  | 318 | Monofluorodichloro methane | CHFCl2 | 0.000 | 290 | 4.559 | 0.836 | 0.708 | -0.076 | 0.118 | 0.119 |
|  | 319 | Monofluorodichloro methane | CHFCl2 | 0.000 | 300 | 4.559 | 0.836 | 0.708 | -0.076 | 0.116 | 0.117 |
|  | 320 | Monofluorodichloro methane | CHFCl2 | 0.000 | 310 | 4.559 | 0.836 | 0.708 | -0.076 | 0.114 | 0.115 |
|  | 321 | Monofluorodichloro methane | CHFCl2 | 0.000 | 320 | 4.559 | 0.836 | 0.708 | -0.076 | 0.112 | 0.114 |
|  | 322 | Monofluorodichloro methane | CHFCl2 | 0.000 | 330 | 4.559 | 0.836 | 0.708 | -0.076 | 0.111 | 0.112 |
|  | 323 | Tetrafluoro dichloro ethane | C2F4Cl2 | 0.000 | 340 | 4.559 | 0.836 | 0.708 | -0.076 | 0.109 | 0.110 |
|  | 324 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 193 | 4.960 | 0.626 | 0.677 | 0.018 | 0.090 | 0.082 |
|  | 325 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 213 | 4.960 | 0.626 | 0.677 | 0.018 | 0.085 | 0.078 |
|  | 326 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 233 | 4.960 | 0.626 | 0.677 | 0.018 | 0.080 | 0.075 |
|  | 327 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 253 | 4.960 | 0.626 | 0.677 | 0.018 | 0.075 | 0.071 |
|  | 328 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 273 | 4.960 | 0.626 | 0.677 | 0.018 | 0.070 | 0.067 |
|  | 329 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 293 | 4.960 | 0.626 | 0.677 | 0.018 | 0.065 | 0.064 |
|  | 330 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 313 | 4.960 | 0.626 | 0.677 | 0.018 | 0.059 | 0.060 |
|  | 331 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 333 | 4.960 | 0.626 | 0.677 | 0.018 | 0.055 | 0.057 |
|  | 332 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 353 | 4.960 | 0.626 | 0.677 | 0.018 | 0.049 | 0.053 |
|  | 333 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 373 | 4.960 | 0.626 | 0.677 | 0.018 | 0.045 | 0.049 |
|  | 334 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 383 | 4.960 | 0.626 | 0.677 | 0.018 | 0.042 | 0.048 |
|  | 335 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 387 | 4.960 | 0.626 | 0.677 | 0.018 | 0.041 | 0.047 |
|  | 336 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 193 | 4.960 | 0.626 | 0.677 | 0.018 | 0.090 | 0.082 |
|  | 337 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 213 | 4.960 | 0.626 | 0.677 | 0.018 | 0.085 | 0.078 |
|  | 338 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 233 | 4.960 | 0.626 | 0.677 | 0.018 | 0.080 | 0.075 |
|  | 339 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 253 | 4.960 | 0.626 | 0.677 | 0.018 | 0.075 | 0.071 |
|  | 340 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 273 | 4.960 | 0.626 | 0.677 | 0.018 | 0.070 | 0.067 |
|  | 341 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 293 | 4.960 | 0.626 | 0.677 | 0.018 | 0.065 | 0.064 |
|  | 342 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 333 | 4.960 | 0.626 | 0.677 | 0.018 | 0.055 | 0.057 |
|  | 343 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 353 | 4.960 | 0.626 | 0.677 | 0.018 | 0.049 | 0.053 |
|  | 344 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 373 | 4.960 | 0.626 | 0.677 | 0.018 | 0.045 | 0.049 |
|  | 345 | Tetrafluoro dichloro ethane | C2F4Cl2 | 1.000 | 383 | 4.960 | 0.626 | 0.677 | 0.018 | 0.042 | 0.048 |
|  | 346 | Tetrachloro ethane | CHCl2CHCl2 | 1.000 | 387 | 4.960 | 0.626 | 0.677 | 0.018 | 0.041 | 0.047 |
|  | 347 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 280 | 5.132 | 0.642 | 0.376 | -0.141 | 0.116 | 0.115 |
|  | 348 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 290 | 5.132 | 0.642 | 0.376 | -0.141 | 0.113 | 0.113 |
|  | 349 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 300 | 5.132 | 0.642 | 0.376 | -0.141 | 0.111 | 0.112 |
|  | 350 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 310 | 5.132 | 0.642 | 0.376 | -0.141 | 0.108 | 0.110 |
|  | 351 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 320 | 5.132 | 0.642 | 0.376 | -0.141 | 0.105 | 0.108 |
|  | 352 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 330 | 5.132 | 0.642 | 0.376 | -0.141 | 0.103 | 0.106 |
|  | 353 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 340 | 5.132 | 0.642 | 0.376 | -0.141 | 0.100 | 0.104 |
|  | 354 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 350 | 5.132 | 0.642 | 0.376 | -0.141 | 0.097 | 0.103 |
|  | 355 | Tetrachloro ethane | CHCl2CHCl2 | 0.000 | 360 | 5.132 | 0.642 | 0.376 | -0.141 | 0.095 | 0.101 |
|  | 356 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 370 | 5.132 | 0.642 | 0.376 | -0.141 | 0.092 | 0.099 |
|  | 357 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 280 | 6.482 | 0.702 | 0.271 | 0.086 | 0.103 | 0.101 |
|  | 358 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 290 | 6.482 | 0.702 | 0.271 | 0.086 | 0.102 | 0.099 |
|  | 359 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 300 | 6.482 | 0.702 | 0.271 | 0.086 | 0.100 | 0.097 |
|  | 360 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 310 | 6.482 | 0.702 | 0.271 | 0.086 | 0.098 | 0.095 |
|  | 361 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 320 | 6.482 | 0.702 | 0.271 | 0.086 | 0.097 | 0.093 |
|  | 362 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 330 | 6.482 | 0.702 | 0.271 | 0.086 | 0.095 | 0.092 |
|  | 363 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 340 | 6.482 | 0.702 | 0.271 | 0.086 | 0.094 | 0.090 |
|  | 364 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 350 | 6.482 | 0.702 | 0.271 | 0.086 | 0.092 | 0.088 |
|  | 365 | 1,2-Dibromo ethane | CH2BrCH2Br | 0.000 | 360 | 6.482 | 0.702 | 0.271 | 0.086 | 0.090 | 0.086 |
|  | 366 | Ethyl iodide | C2H5I | 0.000 | 370 | 6.482 | 0.702 | 0.271 | 0.086 | 0.089 | 0.084 |
|  | 367 | Ethyl iodide | C2H5I | 0.000 | 290 | 7.116 | 0.823 | 0.222 | 0.010 | 0.088 | 0.086 |
|  | 368 | Ethyl iodide | C2H5I | 0.000 | 300 | 7.116 | 0.823 | 0.222 | 0.010 | 0.086 | 0.084 |
|  | 369 | Ethyl iodide | C2H5I | 0.000 | 310 | 7.116 | 0.823 | 0.222 | 0.010 | 0.085 | 0.083 |
|  | 370 | Ethyl iodide | C2H5I | 0.000 | 320 | 7.116 | 0.823 | 0.222 | 0.010 | 0.084 | 0.081 |
|  | 371 | Ethyl iodide | C2H5I | 0.000 | 330 | 7.116 | 0.823 | 0.222 | 0.010 | 0.082 | 0.079 |
|  | 372 | isobutyl iodide | C4H9I | 0.000 | 340 | 7.116 | 0.823 | 0.222 | 0.010 | 0.080 | 0.077 |
|  | 373 | isobutyl iodide | C4H9I | 0.000 | 290 | 7.129 | 0.78 | 0.17 | -0.071 | 0.085 | 0.086 |
|  | 374 | isobutyl iodide | C4H9I | 0.000 | 300 | 7.129 | 0.78 | 0.17 | -0.071 | 0.083 | 0.084 |
|  | 375 | isobutyl iodide | C4H9I | 0.000 | 310 | 7.129 | 0.78 | 0.17 | -0.071 | 0.082 | 0.082 |
|  | 376 | isobutyl iodide | C4H9I | 0.000 | 330 | 7.129 | 0.78 | 0.17 | -0.071 | 0.079 | 0.078 |
|  | 377 | isobutyl iodide | C4H9I | 0.000 | 340 | 7.129 | 0.78 | 0.17 | -0.071 | 0.077 | 0.077 |
|  | 378 | isobutyl iodide | C4H9I | 0.000 | 360 | 7.129 | 0.78 | 0.17 | -0.071 | 0.074 | 0.073 |
|  | 379 | isoamyl iodide | C5H11I | 0.000 | 370 | 7.129 | 0.78 | 0.17 | -0.071 | 0.073 | 0.071 |
|  | 380 | isoamyl iodide | C5H11I | 0.000 | 290 | 7.134 | 0.64 | 0.123 | -0.013 | 0.087 | 0.091 |
|  | 381 | isoamyl iodide | C5H11I | 0.000 | 300 | 7.134 | 0.64 | 0.123 | -0.013 | 0.086 | 0.089 |
|  | 382 | isoamyl iodide | C5H11I | 0.000 | 310 | 7.134 | 0.64 | 0.123 | -0.013 | 0.084 | 0.087 |
|  | 383 | isoamyl iodide | C5H11I | 0.000 | 320 | 7.134 | 0.64 | 0.123 | -0.013 | 0.083 | 0.085 |
|  | 384 | isoamyl iodide | C5H11I | 0.000 | 340 | 7.134 | 0.64 | 0.123 | -0.013 | 0.080 | 0.082 |
|  | 385 | isoamyl iodide | C5H11I | 0.000 | 350 | 7.134 | 0.64 | 0.123 | -0.013 | 0.079 | 0.080 |
|  | 386 | isoamyl iodide | C5H11I | 0.000 | 370 | 7.134 | 0.64 | 0.123 | -0.013 | 0.076 | 0.076 |
|  | 387 | n-heptyl iodide | C7H15I | 0.000 | 380 | 7.134 | 0.64 | 0.123 | -0.013 | 0.075 | 0.075 |
|  | 388 | n-heptyl iodide | C7H15I | 0.000 | 280 | 7.144 | 0.404 | 0.095 | 0.160 | 0.103 | 0.103 |
|  | 389 | n-heptyl iodide | C7H15I | 0.000 | 300 | 7.144 | 0.404 | 0.095 | 0.160 | 0.099 | 0.100 |
|  | 390 | n-heptyl iodide | C7H15I | 0.000 | 320 | 7.144 | 0.404 | 0.095 | 0.160 | 0.096 | 0.096 |
|  | 391 | n-heptyl iodide | C7H15I | 0.000 | 340 | 7.144 | 0.404 | 0.095 | 0.160 | 0.093 | 0.092 |
|  | 392 | n-heptyl iodide | C7H15I | 0.000 | 360 | 7.144 | 0.404 | 0.095 | 0.160 | 0.090 | 0.089 |
|  | 393 | n-heptyl iodide | C7H15I | 0.000 | 380 | 7.144 | 0.404 | 0.095 | 0.160 | 0.087 | 0.085 |
|  | 394 | n-heptyl iodide | C7H15I | 0.000 | 400 | 7.144 | 0.404 | 0.095 | 0.160 | 0.083 | 0.082 |
|  | 395 | n-heptyl iodide | C7H15I | 0.000 | 420 | 7.144 | 0.404 | 0.095 | 0.160 | 0.080 | 0.078 |
|  | 396 | n-heptyl iodide | C7H15I | 0.000 | 440 | 7.144 | 0.404 | 0.095 | 0.160 | 0.077 | 0.074 |
|  | 397 | n-octyl bromide | C8H17Br | 0.000 | 450 | 7.144 | 0.404 | 0.095 | 0.160 | 0.076 | 0.073 |
|  | 398 | n-octyl bromide | C8H17Br | 0.000 | 290 | 5.926 | 0.358 | 0.079 | 0.281 | 0.112 | 0.116 |
|  | 399 | n-octyl bromide | C8H17Br | 0.000 | 310 | 5.926 | 0.358 | 0.079 | 0.281 | 0.110 | 0.112 |
|  | 400 | n-octyl bromide | C8H17Br | 0.000 | 330 | 5.926 | 0.358 | 0.079 | 0.281 | 0.107 | 0.109 |
|  | 401 | n-octyl bromide | C8H17Br | 0.000 | 350 | 5.926 | 0.358 | 0.079 | 0.281 | 0.105 | 0.105 |
|  | 402 | n-octyl bromide | C8H17Br | 0.000 | 370 | 5.926 | 0.358 | 0.079 | 0.281 | 0.102 | 0.102 |
|  | 403 | n-octyl chloride | C8H17Cl | 0.000 | 390 | 5.926 | 0.358 | 0.079 | 0.281 | 0.100 | 0.098 |
|  | 404 | n-octyl chloride | C8H17Cl | 0.000 | 280 | 4.526 | 0.359 | 0.074 | 0.212 | 0.129 | 0.130 |
|  | 405 | n-octyl chloride | C8H17Cl | 0.000 | 300 | 4.526 | 0.359 | 0.074 | 0.212 | 0.127 | 0.126 |
|  | 406 | n-octyl chloride | C8H17Cl | 0.000 | 320 | 4.526 | 0.359 | 0.074 | 0.212 | 0.125 | 0.123 |
|  | 407 | n-octyl chloride | C8H17Cl | 0.000 | 360 | 4.526 | 0.359 | 0.074 | 0.212 | 0.120 | 0.116 |
|  | 408 | n-octyl chloride | C8H17Cl | 0.000 | 380 | 4.526 | 0.359 | 0.074 | 0.212 | 0.118 | 0.112 |
|  | 409 | n-octyl chloride | C8H17Cl | 0.000 | 400 | 4.526 | 0.359 | 0.074 | 0.212 | 0.116 | 0.108 |
|  | 410 | Monofluorodichloro methane | CHFCl2 | 0.000 | 420 | 4.526 | 0.359 | 0.074 | 0.212 | 0.114 | 0.105 |

**Table S2. AD Check of GFA model**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***Set*** | ***No.*** | ***Compound*** | **Formula** | ***Outlier Info.*** |
| **Training set** | 1 | Carbon tetrachloride | CCl4 | - |
|  | 2 | Carbon tetrachloride | CCl4 | - |
|  | 3 | Carbon tetrachloride | CCl4 | - |
|  | 4 | Carbon tetrachloride | CCl4 | - |
|  | 5 | Carbon tetrachloride | CCl4 | - |
|  | 6 | Carbon tetrachloride | CCl4 | - |
|  | 7 | Carbon tetrachloride | CCl4 | - |
|  | 8 | Carbon tetrachloride | CCl4 | - |
|  | 9 | Carbon tetrachloride | CCl4 | - |
|  | 10 | Carbon tetrachloride | CCl4 | - |
|  | 11 | Carbon tetrachloride | CCl4 | - |
|  | 12 | Carbon tetrachloride | CCl4 | - |
|  | 13 | Carbon tetrachloride | CCl4 | - |
|  | 14 | Carbon tetrachloride | CCl4 | - |
|  | 15 | Carbon tetrachloride | CCl4 | - |
|  | 16 | Carbon tetrachloride | CCl4 | - |
|  | 17 | Carbon tetrachloride | CCl4 | - |
|  | 18 | Carbon tetrachloride | CCl4 | - |
|  | 19 | Carbon tetrachloride | CCl4 | - |
|  | 20 | Carbon tetrachloride | CCl4 | - |
|  | 21 | Carbon tetrachloride | CCl4 | - |
|  | 22 | Carbon tetrachloride | CCl4 | - |
|  | 23 | Trifluoromonobromo methane | CF3Br | - |
|  | 24 | Trifluoromonobromo methane | CF3Br | - |
|  | 25 | Trifluoromonobromo methane | CF3Br | - |
|  | 26 | Trifluoromonobromo methane | CF3Br | - |
|  | 27 | Trifluoromonobromo methane | CF3Br | - |
|  | 28 | Trifluoromonobromo methane | CF3Br | - |
|  | 29 | Trifluoromonobromo methane | CF3Br | - |
|  | 30 | Trifluoromonobromo methane | CF3Br | - |
|  | 31 | Trifluoromonobromo methane | CF3Br | - |
|  | 32 | Trifluoromonobromo methane | CF3Br | - |
|  | 33 | Trifluoromonobromo methane | CF3Br | - |
|  | 34 | Trifluoromonobromo methane | CF3Br | - |
|  | 35 | Trifluoromonobromo methane | CF3Br | - |
|  | 36 | Trifluoromonobromo methane | CF3Br | - |
|  | 37 | Trifluoromonobromo methane | CF3Br | - |
|  | 38 | Trifluoromonobromo methane | CF3Br | - |
|  | 39 | Trifluoromonobromo methane | CF3Br | - |
|  | 40 | Trifluoromonobromo methane | CF3Br | - |
|  | 41 | Trifluoromonobromo methane | CF3Br | - |
|  | 42 | Trifluoromonobromo methane | CF3Br | - |
|  | 43 | Trifluoromonobromo methane | CF3Br | - |
|  | 44 | Trifluoromonobromo methane | CF3Br | - |
|  | 45 | Trifluoromonobromo methane | CF3Br | - |
|  | 46 | Trifluoromonobromo methane | CF3Br | - |
|  | 47 | Bromoform | CHBr3 | - |
|  | 48 | Bromoform | CHBr3 | - |
|  | 49 | Bromoform | CHBr3 | - |
|  | 50 | Bromoform | CHBr3 | - |
|  | 51 | Bromoform | CHBr3 | - |
|  | 52 | Bromoform | CHBr3 | - |
|  | 53 | Bromoform | CHBr3 | - |
|  | 54 | Bromoform | CHBr3 | - |
|  | 55 | Bromoform | CHBr3 | - |
|  | 56 | Monofluorodichloro methane | CHFCl2 | - |
|  | 57 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 58 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 59 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 60 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 61 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 62 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 63 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 64 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 65 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 66 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 67 | Tetrachloro ethylene | CCl2CCl2 | - |
|  | 68 | Ethyl bromide | C2H5Br | - |
|  | 69 | Ethyl bromide | C2H5Br | - |
|  | 70 | Ethyl bromide | C2H5Br | - |
|  | 71 | Ethyl bromide | C2H5Br | - |
|  | 72 | Ethyl bromide | C2H5Br | - |
|  | 73 | Ethyl bromide | C2H5Br | - |
|  | 74 | Ethyl bromide | C2H5Br | - |
|  | 75 | Ethyl bromide | C2H5Br | - |
|  | 76 | Ethyl bromide | C2H5Br | - |
|  | 77 | Ethyl bromide | C2H5Br | - |
|  | 78 | Ethyl bromide | C2H5Br | - |
|  | 79 | Ethyl bromide | C2H5Br | - |
|  | 80 | Ethyl iodide | C2H5I | - |
|  | 81 | Octafluoro propane | C3F8 | - |
|  | 82 | Octafluoro propane | C3F8 | - |
|  | 83 | Octafluoro propane | C3F8 | - |
|  | 84 | Octafluoro propane | C3F8 | - |
|  | 85 | Octafluoro propane | C3F8 | - |
|  | 86 | Octafluoro propane | C3F8 | - |
|  | 87 | Octafluoro propane | C3F8 | - |
|  | 88 | Octafluoro propane | C3F8 | - |
|  | 89 | Octafluoro propane | C3F8 | - |
|  | 90 | Octafluoro propane | C3F8 | - |
|  | 91 | Octafluoro propane | C3F8 | - |
|  | 92 | Octafluoro propane | C3F8 | - |
|  | 93 | Octafluoro propane | C3F8 | - |
|  | 94 | Octafluoro propane | C3F8 | - |
|  | 95 | Octafluoro propane | C3F8 | - |
|  | 96 | n-Propyl bromide | C3H7Br | - |
|  | 97 | n-Propyl bromide | C3H7Br | - |
|  | 98 | n-Propyl bromide | C3H7Br | - |
|  | 99 | n-Propyl bromide | C3H7Br | - |
|  | 100 | n-Propyl bromide | C3H7Br | - |
|  | 101 | n-Propyl bromide | C3H7Br | - |
|  | 102 | n-Propyl bromide | C3H7Br | - |
|  | 103 | n-Propyl bromide | C3H7Br | - |
|  | 104 | n-Propyl bromide | C3H7Br | - |
|  | 105 | n-Propyl bromide | C3H7Br | - |
|  | 106 | n-Propyl bromide | C3H7Br | - |
|  | 107 | n-Propyl iodide | C3H7I | - |
|  | 108 | n-Propyl iodide | C3H7I | - |
|  | 109 | n-Propyl iodide | C3H7I | - |
|  | 110 | n-Propyl iodide | C3H7I | - |
|  | 111 | n-Propyl iodide | C3H7I | - |
|  | 112 | n-Propyl iodide | C3H7I | - |
|  | 113 | n-Propyl iodide | C3H7I | - |
|  | 114 | n-Propyl iodide | C3H7I | - |
|  | 115 | butyl bromide | C4H9Br | - |
|  | 116 | butyl bromide | C4H9Br | - |
|  | 117 | butyl bromide | C4H9Br | - |
|  | 118 | butyl bromide | C4H9Br | - |
|  | 119 | butyl bromide | C4H9Br | - |
|  | 120 | butyl bromide | C4H9Br | - |
|  | 121 | butyl bromide | C4H9Br | - |
|  | 122 | butyl bromide | C4H9Br | - |
|  | 123 | butyl bromide | C4H9Br | - |
|  | 124 | butyl bromide | C4H9Br | - |
|  | 125 | butyl bromide | C4H9Br | - |
|  | 126 | butyl bromide | C4H9Br | - |
|  | 127 | butyl bromide | C4H9Br | - |
|  | 128 | butyl bromide | C4H9Br | - |
|  | 129 | butyl bromide | C4H9Br | - |
|  | 130 | butyl bromide | C4H9Br | - |
|  | 131 | isobutyl bromide | C4H9Br | - |
|  | 132 | isobutyl bromide | C4H9Br | - |
|  | 133 | isobutyl bromide | C4H9Br | - |
|  | 134 | isobutyl bromide | C4H9Br | - |
|  | 135 | isobutyl bromide | C4H9Br | - |
|  | 136 | isobutyl bromide | C4H9Br | - |
|  | 137 | isobutyl bromide | C4H9Br | - |
|  | 138 | isobutyl bromide | C4H9Br | - |
|  | 139 | butyl iodide | C4H9I | - |
|  | 140 | butyl iodide | C4H9I | - |
|  | 141 | butyl iodide | C4H9I | - |
|  | 142 | butyl iodide | C4H9I | - |
|  | 143 | butyl iodide | C4H9I | - |
|  | 144 | butyl iodide | C4H9I | - |
|  | 145 | butyl iodide | C4H9I | - |
|  | 146 | butyl iodide | C4H9I | - |
|  | 147 | butyl iodide | C4H9I | - |
|  | 148 | butyl iodide | C4H9I | - |
|  | 149 | butyl iodide | C4H9I | - |
|  | 150 | isobutyl iodide | C4H9I | - |
|  | 151 | isobutyl iodide | C4H9I | - |
|  | 152 | isobutyl iodide | C4H9I | - |
|  | 153 | n-amyl bromide | C5H11Br | - |
|  | 154 | n-amyl bromide | C5H11Br | - |
|  | 155 | n-amyl bromide | C5H11Br | - |
|  | 156 | n-amyl bromide | C5H11Br | - |
|  | 157 | n-amyl bromide | C5H11Br | - |
|  | 158 | n-amyl bromide | C5H11Br | - |
|  | 159 | n-amyl bromide | C5H11Br | - |
|  | 160 | n-amyl bromide | C5H11Br | - |
|  | 161 | n-amyl bromide | C5H11Br | - |
|  | 162 | n-amyl bromide | C5H11Br | - |
|  | 163 | n-amyl bromide | C5H11Br | - |
|  | 164 | n-amyl bromide | C5H11Br | - |
|  | 165 | n-amyl bromide | C5H11Br | - |
|  | 166 | n-amyl bromide | C5H11Br | - |
|  | 167 | n-amyl bromide | C5H11Br | - |
|  | 168 | n-amyl bromide | C5H11Br | - |
|  | 169 | n-amyl bromide | C5H11Br | - |
|  | 170 | n-amyl chloride | C5H11Cl | - |
|  | 171 | n-amyl chloride | C5H11Cl | - |
|  | 172 | n-amyl chloride | C5H11Cl | - |
|  | 173 | n-amyl chloride | C5H11Cl | - |
|  | 174 | n-amyl chloride | C5H11Cl | - |
|  | 175 | n-amyl chloride | C5H11Cl | - |
|  | 176 | n-amyl chloride | C5H11Cl | - |
|  | 177 | n-amyl chloride | C5H11Cl | - |
|  | 178 | n-amyl chloride | C5H11Cl | - |
|  | 179 | n-amyl iodide | C5H11I | - |
|  | 180 | n-amyl iodide | C5H11I | - |
|  | 181 | n-amyl iodide | C5H11I | - |
|  | 182 | n-amyl iodide | C5H11I | - |
|  | 183 | n-amyl iodide | C5H11I | - |
|  | 184 | n-amyl iodide | C5H11I | - |
|  | 185 | n-amyl iodide | C5H11I | - |
|  | 186 | n-amyl iodide | C5H11I | - |
|  | 187 | n-amyl iodide | C5H11I | - |
|  | 188 | n-amyl iodide | C5H11I | - |
|  | 189 | n-amyl iodide | C5H11I | - |
|  | 190 | n-amyl iodide | C5H11I | - |
|  | 191 | n-amyl iodide | C5H11I | - |
|  | 192 | n-amyl iodide | C5H11I | - |
|  | 193 | isoamyl iodide | C5H11I | - |
|  | 194 | isoamyl iodide | C5H11I | - |
|  | 195 | isoamyl iodide | C5H11I | - |
|  | 196 | isoamyl iodide | C5H11I | - |
|  | 197 | n-bromo hexane | C6H13Br | - |
|  | 198 | n-bromo hexane | C6H13Br | - |
|  | 199 | n-bromo hexane | C6H13Br | - |
|  | 200 | n-bromo hexane | C6H13Br | - |
|  | 201 | n-bromo hexane | C6H13Br | - |
|  | 202 | n-bromo hexane | C6H13Br | - |
|  | 203 | n-bromo hexane | C6H13Br | - |
|  | 204 | n-bromo hexane | C6H13Br | - |
|  | 205 | n-bromo hexane | C6H13Br | - |
|  | 206 | n-bromo hexane | C6H13Br | - |
|  | 207 | n-bromo hexane | C6H13Br | - |
|  | 208 | n-bromo hexane | C6H13Br | - |
|  | 209 | n-bromo hexane | C6H13Br | - |
|  | 210 | n-bromo hexane | C6H13Br | - |
|  | 211 | n-bromo hexane | C6H13Br | - |
|  | 212 | n-bromo hexane | C6H13Br | - |
|  | 213 | n-bromo hexane | C6H13Br | - |
|  | 214 | n-hexyl iodide | C6H13I | - |
|  | 215 | n-hexyl iodide | C6H13I | - |
|  | 216 | n-hexyl iodide | C6H13I | - |
|  | 217 | n-hexyl iodide | C6H13I | - |
|  | 218 | n-hexyl iodide | C6H13I | - |
|  | 219 | n-hexyl iodide | C6H13I | - |
|  | 220 | n-hexyl iodide | C6H13I | - |
|  | 221 | n-hexyl iodide | C6H13I | - |
|  | 222 | n-perfluoro heptane | C7F16 | - |
|  | 223 | n-perfluoro heptane | C7F16 | - |
|  | 224 | n-perfluoro heptane | C7F16 | - |
|  | 225 | n-perfluoro heptane | C7F16 | - |
|  | 226 | n-perfluoro heptane | C7F16 | - |
|  | 227 | n-perfluoro heptane | C7F16 | - |
|  | 228 | n-perfluoro heptane | C7F16 | - |
|  | 229 | n-perfluoro heptane | C7F16 | - |
|  | 230 | 1-bromo heptane | C7H15Br | - |
|  | 231 | 1-bromo heptane | C7H15Br | - |
|  | 232 | 1-bromo heptane | C7H15Br | - |
|  | 233 | 1-bromo heptane | C7H15Br | - |
|  | 234 | 1-bromo heptane | C7H15Br | - |
|  | 235 | 1-bromo heptane | C7H15Br | - |
|  | 236 | 1-bromo heptane | C7H15Br | - |
|  | 237 | 1-bromo heptane | C7H15Br | - |
|  | 238 | 1-chloro heptane | C7H15Cl | - |
|  | 239 | 1-chloro heptane | C7H15Cl | - |
|  | 240 | 1-chloro heptane | C7H15Cl | - |
|  | 241 | 1-chloro heptane | C7H15Cl | - |
|  | 242 | 1-chloro heptane | C7H15Cl | - |
|  | 243 | 1-chloro heptane | C7H15Cl | - |
|  | 244 | 1-chloro heptane | C7H15Cl | - |
|  | 245 | 1-chloro heptane | C7H15Cl | - |
|  | 246 | decyl bromide | C10H21Br | - |
|  | 247 | decyl bromide | C10H21Br | - |
|  | 248 | decyl bromide | C10H21Br | - |
|  | 249 | decyl bromide | C10H21Br | - |
|  | 250 | decyl bromide | C10H21Br | - |
|  | 251 | decyl bromide | C10H21Br | - |
|  | 252 | decyl bromide | C10H21Br | - |
|  | 253 | isodecyl bromide | C10H21Br | - |
|  | 254 | isodecyl bromide | C10H21Br | - |
|  | 255 | isodecyl bromide | C10H21Br | - |
|  | 256 | isodecyl bromide | C10H21Br | - |
|  | 257 | isodecyl bromide | C10H21Br | - |
|  | 258 | isodecyl chloride | C10H21Cl | - |
|  | 259 | isodecyl chloride | C10H21Cl | - |
|  | 260 | isodecyl chloride | C10H21Cl | - |
|  | 261 | n-perfluoro octane | C8F18 | - |
|  | 262 | n-perfluoro octane | C8F18 | - |
|  | 263 | n-perfluoro octane | C8F18 | - |
|  | 264 | n-perfluoro octane | C8F18 | - |
|  | 265 | n-perfluoro octane | C8F18 | - |
|  | 266 | n-perfluoro octane | C8F18 | - |
|  | 267 | n-perfluoro octane | C8F18 | - |
|  | 268 | n-octyl chloride | C8H17Cl | - |
|  | 269 | n-octyl iodide | C8H17I | - |
|  | 270 | n-octyl iodide | C8H17I | - |
|  | 271 | n-octyl iodide | C8H17I | - |
|  | 272 | n-octyl iodide | C8H17I | - |
|  | 273 | n-octyl iodide | C8H17I | - |
|  | 274 | n-octyl iodide | C8H17I | - |
|  | 275 | n-octyl iodide | C8H17I | - |
|  | 276 | n-octyl iodide | C8H17I | - |
|  | 277 | n-octyl iodide | C8H17I | - |
|  | 278 | n-octyl iodide | C8H17I | - |
|  | 279 | n-nonyl bromide | C9H19Br | - |
|  | 280 | n-nonyl bromide | C9H19Br | - |
|  | 281 | n-nonyl bromide | C9H19Br | - |
|  | 282 | n-nonyl bromide | C9H19Br | - |
|  | 283 | n-nonyl bromide | C9H19Br | - |
|  | 284 | n-nonyl bromide | C9H19Br | - |
|  | 285 | n-nonyl bromide | C9H19Br | - |
|  | 286 | n-nonyl bromide | C9H19Br | - |
|  | 287 | n-nonyl bromide | C9H19Br | - |
|  | 288 | n-nonyl chloride | C9H19Cl | - |
|  | 289 | n-nonyl chloride | C9H19Cl | - |
|  | 290 | n-nonyl chloride | C9H19Cl | - |
|  | 291 | n-nonyl chloride | C9H19Cl | - |
|  | 292 | n-nonyl chloride | C9H19Cl | - |
|  | 293 | n-nonyl chloride | C9H19Cl | - |
|  | 294 | n-nonyl chloride | C9H19Cl | - |
|  | 295 | n-nonyl chloride | C9H19Cl | - |
|  | 296 | n-nonyl chloride | C9H19Cl | - |
|  | 297 | n-nonyl chloride | C9H19Cl | - |
|  | 298 | n-nonyl iodide | C9H19I | - |
|  | 299 | n-nonyl iodide | C9H19I | - |
|  | 300 | n-nonyl iodide | C9H19I | - |
|  | 301 | n-nonyl iodide | C9H19I | - |
|  | 302 | n-nonyl iodide | C9H19I | - |
|  | 303 | n-nonyl iodide | C9H19I | - |
|  | 304 | n-nonyl iodide | C9H19I | - |
|  | 305 | n-nonyl iodide | C9H19I | - |
|  | 306 | n-nonyl iodide | C9H19I | - |
|  | 307 | n-nonyl iodide | C9H19I | - |
| **Prediction set** | 308 | Monofluorodichloro methane | CHFCl2 | - |
|  | 309 | Monofluorodichloro methane | CHFCl2 | - |
|  | 310 | Monofluorodichloro methane | CHFCl2 | - |
|  | 311 | Monofluorodichloro methane | CHFCl2 | - |
|  | 312 | Monofluorodichloro methane | CHFCl2 | - |
|  | 313 | Monofluorodichloro methane | CHFCl2 | - |
|  | 314 | Monofluorodichloro methane | CHFCl2 | - |
|  | 315 | Monofluorodichloro methane | CHFCl2 | - |
|  | 316 | Monofluorodichloro methane | CHFCl2 | - |
|  | 317 | Monofluorodichloro methane | CHFCl2 | - |
|  | 318 | Monofluorodichloro methane | CHFCl2 | - |
|  | 319 | Monofluorodichloro methane | CHFCl2 | - |
|  | 320 | Monofluorodichloro methane | CHFCl2 | - |
|  | 321 | Monofluorodichloro methane | CHFCl2 | - |
|  | 322 | Monofluorodichloro methane | CHFCl2 | - |
|  | 323 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 324 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 325 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 326 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 327 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 328 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 329 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 330 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 331 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 332 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 333 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 334 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 335 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 336 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 337 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 338 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 339 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 340 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 341 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 342 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 343 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 344 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 345 | Tetrafluoro dichloro ethane | C2F4Cl2 | - |
|  | 346 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 347 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 348 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 349 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 350 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 351 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 352 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 353 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 354 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 355 | Tetrachloro ethane | CHCl2CHCl2 | - |
|  | 356 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 357 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 358 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 359 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 360 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 361 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 362 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 363 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 364 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 365 | 1,2-Dibromo ethane | CH2BrCH2Br | - |
|  | 366 | Ethyl iodide | C2H5I | - |
|  | 367 | Ethyl iodide | C2H5I | - |
|  | 368 | Ethyl iodide | C2H5I | - |
|  | 369 | Ethyl iodide | C2H5I | - |
|  | 370 | Ethyl iodide | C2H5I | - |
|  | 371 | Ethyl iodide | C2H5I | - |
|  | 372 | isobutyl iodide | C4H9I | - |
|  | 373 | isobutyl iodide | C4H9I | - |
|  | 374 | isobutyl iodide | C4H9I | - |
|  | 375 | isobutyl iodide | C4H9I | - |
|  | 376 | isobutyl iodide | C4H9I | - |
|  | 377 | isobutyl iodide | C4H9I | - |
|  | 378 | isobutyl iodide | C4H9I | - |
|  | 379 | isoamyl iodide | C5H11I | - |
|  | 380 | isoamyl iodide | C5H11I | - |
|  | 381 | isoamyl iodide | C5H11I | - |
|  | 382 | isoamyl iodide | C5H11I | - |
|  | 383 | isoamyl iodide | C5H11I | - |
|  | 384 | isoamyl iodide | C5H11I | - |
|  | 385 | isoamyl iodide | C5H11I | - |
|  | 386 | isoamyl iodide | C5H11I | - |
|  | 387 | n-heptyl iodide | C7H15I | - |
|  | 388 | n-heptyl iodide | C7H15I | - |
|  | 389 | n-heptyl iodide | C7H15I | - |
|  | 390 | n-heptyl iodide | C7H15I | - |
|  | 391 | n-heptyl iodide | C7H15I | - |
|  | 392 | n-heptyl iodide | C7H15I | - |
|  | 393 | n-heptyl iodide | C7H15I | - |
|  | 394 | n-heptyl iodide | C7H15I | - |
|  | 395 | n-heptyl iodide | C7H15I | - |
|  | 396 | n-heptyl iodide | C7H15I | - |
|  | 397 | n-octyl bromide | C8H17Br | - |
|  | 398 | n-octyl bromide | C8H17Br | - |
|  | 399 | n-octyl bromide | C8H17Br | - |
|  | 400 | n-octyl bromide | C8H17Br | - |
|  | 401 | n-octyl bromide | C8H17Br | - |
|  | 402 | n-octyl bromide | C8H17Br | - |
|  | 403 | n-octyl chloride | C8H17Cl | - |
|  | 404 | n-octyl chloride | C8H17Cl | - |
|  | 405 | n-octyl chloride | C8H17Cl | - |
|  | 406 | n-octyl chloride | C8H17Cl | - |
|  | 407 | n-octyl chloride | C8H17Cl | - |
|  | 408 | n-octyl chloride | C8H17Cl | - |
|  | 409 | n-octyl chloride | C8H17Cl | - |
|  | 410 | Monofluorodichloro methane | CHFCl2 | - |

**Table S3. Prediction of some halogenated alkanes not involved in the present study.**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Compound** | ***B02[F-F]*** | ***SpMaxA\_AEA(ri)*** | ***SM3\_B(m)*** | ***RPCG*** | ***Mor11v*** | ***T*** | ***λ*exp/**  **(W/m·K)** | **GFA-MLR-*λ*cal/**  **(W/m·K)** | **Residuals of**  **GFA-MLR** |
| 1 | Chloropropane | 0.000 | 0.766 | 4.049 | 0.169 | -0.102 | 280 | 0.121 | 0.111 | 0.010 |
| 2 | Chloropropane | 0.000 | 0.766 | 4.049 | 0.169 | -0.102 | 290 | 0.118 | 0.109 | 0.009 |
| 3 | Chloropropane | 0.000 | 0.766 | 4.049 | 0.169 | -0.102 | 300 | 0.116 | 0.107 | 0.009 |
| 4 | Chloropropane | 0.000 | 0.766 | 4.049 | 0.169 | -0.102 | 310 | 0.114 | 0.105 | 0.009 |
| 5 | Trifluoromethane | 1.000 | 0.900 | 3.738 | 0.776 | 0.143 | 280 | 0.0725 | 0.065 | 0.007 |
| 6 | Trifluoromethane | 1.000 | 0.900 | 3.738 | 0.776 | 0.143 | 290 | 0.0655 | 0.063 | 0.002 |
| 7 | Trifluoromethane | 1.000 | 0.900 | 3.738 | 0.776 | 0.143 | 300 | 0.0585 | 0.061 | -0.003 |
| 8 | Trifluoromethane | 1.000 | 0.900 | 3.738 | 0.776 | 0.143 | 310 | 0.0515 | 0.059 | -0.008 |
| 9 | Trichloromethane | 0.000 | 0.800 | 4.806 | 0.681 | -0.263 | 280 | 0.119 | 0.111 | 0.008 |
| 10 | Trichloromethane | 0.000 | 0.800 | 4.806 | 0.681 | -0.263 | 290 | 0.118 | 0.109 | 0.009 |
| 11 | Trichloromethane | 0.000 | 0.800 | 4.806 | 0.681 | -0.263 | 300 | 0.116 | 0.107 | 0.009 |
| 12 | Trichloromethane | 0.000 | 0.800 | 4.806 | 0.681 | -0.263 | 310 | 0.114 | 0.105 | 0.009 |