QSPR Flash Point Prediction of Solvents Using Topological Indices for Application in Computer Aided Molecular Design. Suhani J. Patel, Dedy Ng, and M. Sam Mannan\*

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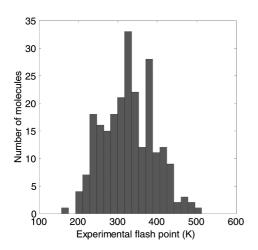
This revision corrects an unfortunate mistake in compiling data for experimental flash point values for hydrocarbons published in Table 4 (pages 7381-7384). The ensuing changes to the text of the publication are on the following pages: page 7378 in the Abstract "The neural network model showed higher accuracy (training set, r = 0.939,  $R^2 = 0.883$ )"; page 7380 in the Methodology section "(range of flash points = 513.15 K - 157.15 K = 356 K, standard deviation = 64.81 K)"; and page 7385 in the Results and Discussion "Upon using the entire data set for multiple linear regression analysis, poor accuracy was obtained ( $R^2 = 0.479$ , r = 0.692)", "The average absolute deviation is 20.819 K, the average absolute relative deviation is 6.57%, and the average bias is -0.21% for the data set using MLR", "A 16:6:1 network (consisting of 16 input nodes as given in

Table 2, one output node, and one hidden layer with 6 nodes)", "The average absolute relative deviation is 5.35%, the average absolute deviation is 16.08 K, and the average percent bias is -0.22% for the complete data set using ANN".

The ensuing changes for figures in the publication are Figures 3–5 (on page 7379), Figure 6 (on page 7380), and Figure 7 (on page 7385).

The ensuing changes for tables in the publication are Tables 1 and 3 (on page 7380) and Table 4 (on pages 7381–7384)

The authors gratefully acknowledge Mr. Max Bernhardt and Dr. Andreas Klamt (Universität Regensburg, Germany), who found the issues with the reported flash point values and kindly brought these problems to our attention.



**Figure 3.** Distribution of flash point values in data set (n = 236).

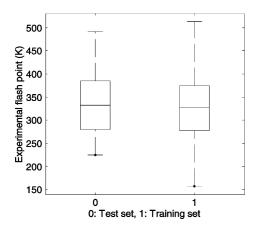


Figure 4. Box plots of test set and training set.

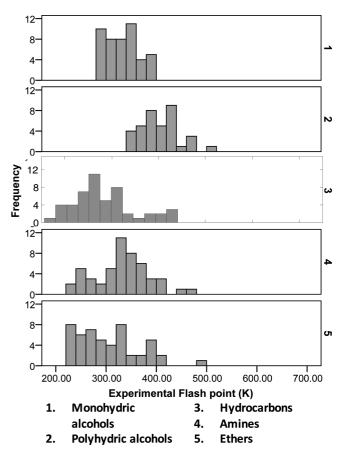


Figure 5. Distribution of flash point values for each class.

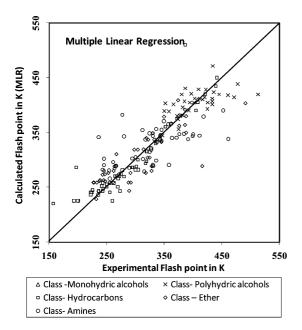


Figure 6. Plot of calculated versus experimental values of flash point using MLR (graph depicts correlations from Table 1 for all classes).

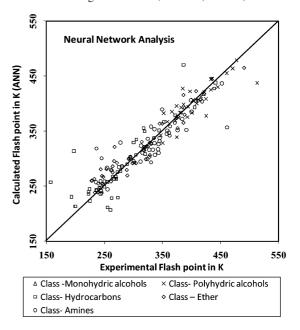


Figure 7. Plot of calculated versus experimental values of flash point using

Table 1. Results of Multiple Linear Regression on Different Classes of Solvents for Flash Point Prediction<sup>a</sup>

|                     |   | training set |       |                     | test set |       |       |
|---------------------|---|--------------|-------|---------------------|----------|-------|-------|
| class of solvents   | equation  | r            | $R^2$ | R <sup>2</sup> (CV) | F        | r     | $R^2$ |
| monohydric alcohols | $T_{\rm f} = 9.248(SC:2) - 34.953(^3\chi_{\rm cluster}) + 286.053$  | 0.925        | 0.855 | 0.613               | 109.06   | 0.933 | 0.870 |
| polyhydric alcohols | $T_{\rm f} = 13.064(^2\kappa) - 8.665(^3\kappa) + 385.328$          | 0.608        | 0.370 |                     | 7.62     | 0.500 | 0.251 |
| hydrocarbons        | $T_{\rm f} = 29.929(^1\chi) - 105.054$                              | 0.881        | 0.776 | 0.696               | 132.15   | 0.792 | 0.628 |
| amines              | $T_{\rm f} = 50.264(^{1}\chi) - 31.887(^{2}\chi_{\rm v}) + 210.783$ | 0.691        | 0.477 | 0.22                | 16.89    | 0.396 | 0.157 |
| ethers              | $T_{\rm f} = 30.045(^{1}\chi) + 186.184$                            | 0.825        | 0.680 | 0.600               | 80.75    | 0.875 | 0.770 |

 $<sup>^</sup>aR^2 = \text{coefficient}$  of determination; r = correlation coefficient;  $R^2(\text{CV}) = R^2$  for the cross validation set, F = Fisher test statistic; SC:2 = subgraph counts (second order): path;  $^3\chi_{\text{cluster}} = \text{chi}(3)$ : cluster;  $^n\kappa = \text{kappa-}n$ ;  $^n\chi = \text{chi}(n)$ ;  $^2\chi_{\text{v}} = \text{chi}(2)$  (valence modified).

Table 3. Results of Neural Network Analysis for Flash Point Prediction (n = 236, Network Configuration =16:6:1)

|              | r     | $R^2$ | $R^2(CV)$ |
|--------------|-------|-------|-----------|
| training set | 0.940 | 0.883 | 0.638     |
| test set     | 0.878 | 0.772 | 0.664     |

Table 4. Solvent Data Set with Experimental and Predicted (MLR and ANN) Flash Point

| Class   Monohydric Alcohols   Class   Monohydric Alcohols   Class   Monohydric Alcohols   Class   Cl   |     |   |                              | $T_{\rm f}$ (predic | cted) (K) |
|--|-----|---|------------------------------|---------------------|-----------|
| methanol   | no. | iupac/cas name  | $T_{\rm f}({\rm exptl})$ (K) | MLR                 | ANN       |
| chanol   |     | Class: Monohydric Alcohol                                     | s                            |                     |           |
| Description   Propriet   Propri   | 1   | methanol  | 283.706                      | 286.053             | 285.091   |
| bottom-2-ol   295.372   308.776   301.045     5  | 2   | ethanol   | 286.483                      | 295.302             | 281.885   |
| 2  | 3   | propan-1-ol   | 298.15                       | 304.55              | 274.462   |
| 6 2-methylpropan-2-ol 284_261 271.635 283.836 7 pentan-2-ol 313,706 318,024 285,256 8 2-methylbratura-1-ol 294_261 296_24 288,576 9 hexnar-1-ol 331,186 334,447 322,1632 10 2-ctrip/thanar-1-ol 331,186 334,447 322,531 11 2-cmethylpropan-2-ol 331,186 334,447 322,531 12 cmethylpropan-2-ol 377,394 369_287 371,028 13 dexart-1-ol 377,394 369_287 371,028 14 phenylmethanol 377,394 369_287 371,028 15 4-ktydroxy4-methylpentan-2-one 323,772 309,714 348,755 16 2-larylmethanol 373,306 361,51 366,481 352,944 17 2-methylpropanoic acid (3-hydroxy-2,2,4-trimethylpenyl) ester 331,15 366,481 382,941 18 1-chloropropan-2-ol 386,15 336,521 383,778 19 1,4-dibromolutian-2-ol 386,15 336,521 383,778 21 heptan-1-ol 386,15 341,542 372,722 321,81 22 heptan-1-ol 386,15 341,542 372,722 321,81 23 1-methoxytropan-2-ol 341,15 372,727 321,81 24 cctan-1-ol 346,15 340,542 333,298 25 (272-2,4-dillydroxy-N/3-hydroxypropyl)-3,3-dimethylbutanamide 386,15 302,489 333,53 26 (272-2,4-dillydroxy-N/3-hydroxypropyl)-3,3-dimethylbutanamide 386,15 302,489 333,53 36 4-methylpentan-1-ol 331,15 322,204 305,933 37 2-ctan-1-ol 331,15 322,204 305,933 38 340,470 333,15 351,918 333,133 39 30 4-methylpentan-1-ol 331,15 322,204 305,933 30 4-methylpentan-1-ol 330,15 334,407 325,511 31 2-methylputan-1-ol 330,15 344,407 325,511 31 2-methylputan-1-ol 330,15 344,407 325,511 31 32-dethylbutan-1-ol 330,15 344,407 325,511 31 32-dethylbutan-1-ol 330,15 344,407 325,511 31 32-dethylputan-1-ol 330,15 334,407 325,511 31 32-dethylbutan-1-ol 330,15 334,407 325,511 32 32-dethylbutan-1-ol 330,15 344,407 325,511 33 32-dethylbutan-1-ol 330,15 344,407 325,511 34 2-dethylbutan-1-ol 330,15 344,407 325,511 35 32-dethylbutan-1-ol 330,15 344,407 325,511 36 32-dethylbutan-1-ol 340,15 340,15 340,15 340,15 340,15 340,15 340,15 34 | 4   | butan-2-ol  | 295.372                      | 308.776             | 301.044   |
| 8 2 - methylbutan-2-ol   | 5   | 2-methylpropan-1-ol   | 303.15                       | 308.776             |           |
| 8  |     | 2-methylpropan-2-ol   |                              | 271.635             |           |
| 10   2-chtylbutan-lol  |     | 1   |                              |                     |           |
| 10   2-chtylbutan-1-ol   331,483   334,407   325,531   11   coctum-2-ol   358,15   345,769   347,779   12   nonan-1-ol   358,15   360,038   357,757   357,759   360,287   371,028   371,028   377,759   360,287   371,028   371,   |     |   |                              |                     |           |
| 11   |     |   |                              |                     |           |
| 12   |     |   |                              |                     |           |
| 13   decan-1-ol   377,594   309,287   371,028   14   4   4   4   4   4   4   5   5   5   |     |   |                              |                     |           |
| 14   phenylmethanol   373,706   302,152   354,812     15   4-hydroxy4-methylpentan-2-one   325,372   309,714   348,755     16   2-furylmethanol   356,483   352,904   350,476     17   2-methylpropanoic acid (3-hydroxy-2,2,4-trimethylpentyl) ester   393,15   306,876   307,247     18   1-chloropropan-2-ol   324,15   308,776   307,247     19   1-chloropropan-2-ol   332,15   336,521   333,879     20   hoptan-2-ol   340,15   341,45   332,95     21   hoptan-1-ol   341,15   327,272   331,879     22   hoxan-2-ol   341,15   327,272   331,879     23   hoxan-2-ol   341,15   327,272   331,879     24   methoxypropan-2-ol   368,15   318,024   333,879     25   (27-2,4-dihydroxy-4/(3-hydroxypropyl)-3,3-dimethylbutanamide   368,15   302,489   347,242     25   corp1-a-3-ol   341,15   322,204   309,379     26   perian-3-ol   341,15   322,204   309,379     27   oct   -ma-3-ol   341,15   349,948   367,998     28   2,2-t-influorechamol   333,15   331,18   333,423     30   4-methylpentan-1-ol   331,15   322,215   336,7998     30   2-methylbutan-2-ol   293,15   296,24   306,375     31   2-methylbutan-1-ol   330,15   334,407   332,531     32   33,3-dimethylbutan-1-ol   330,15   334,407   332,531     33   2-ethylbutan-1-ol   330,15   334,407   332,531     34   2-ethylbutan-1-ol   330,15   334,407   332,531     35   2,2-d-trimothylpentan-1-ol   333,15   331,22   325,312     37   4   4   4   4   5   4   4   5   4   4  |     |   |                              |                     |           |
| 15   |     |   |                              |                     |           |
| 16   2-fury/methanol   356,483   352,904   356,476     17   2-methy/propanoic acid (3-hydroxy-2,2,4-trimethy/pentyl) ester   331,15   396,931   378,536     18   1-chtoropropan-2-ol   324,15   308,776   307,247     19   1,4-diffromobulan-2-ol   386,15   331,452   385,770     20   heptan-1-ol   346,15   341,542   332,572     21   heptan-1-ol   346,15   341,542   332,572     22   hexan-2-ol   314,15   327,272   321,81     31   1-methoxypropan-2-ol   306,15   318,024   333,3379     42   octan-1-ol   354,15   350,79   346,454     25   (2p-2,4-diffydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutanamide   386,15   392,489   472,342     26   pentan-3-ol   311,15   342,249   472,342     27   oct-1-en-3-ol   311,15   342,249   472,342     28   2.2,2-trifithorocthanol   302,15   290,24   306,593     29   2.3,4-trimethylpentan-1-ol   333,15   31,918   330,343     30   4-methylpentan-2-ol   314,15   322,251   316,174     29   2.3,4-trimethylpentan-1-ol   330,15   334,407   325,313     31   2-methylbutan-1-ol   330,15   334,407   325,313     32   2-thylbutan-1-ol   330,15   334,407   325,313     33   2-thylbutan-1-ol   330,15   334,407   325,314     34   2-thylbutan-1-ol   330,15   334,407   325,314     35   2.2,4-trimethylpentan-1-ol   330,15   334,407   325,314     37   2-thylbutan-1-ol   330,15   330,348   317,401     38   38   38   38   38   38   38     39   39   38   38   38   38   38     30   30   30   30   30   30   30  |     |   |                              |                     |           |
| 17   2-methylpropancie acid (3-hydroxy-2,2,4-trimethylpentyl) ester   393,15   396,931   378,539     18   1.4-difromobutan-2-ol   324,15   330,776   307,247     19   1.4-difromobutan-2-ol   336,15   331,452   385,71     10   heptan-2-ol   346,15   341,542   332,95     11   heptan-1-ol   346,15   341,542   332,95     12   heptan-1-ol   346,15   341,542   332,95     13   heptan-1-ol   346,15   318,024   332,35     15   solidary   327,272   321,81     23   1-methoxypropan-2-ol   306,15   318,024   333,533     24   octan-1-ol   354,15   350,79   346,45     25   (2x)-2,4-dihydroxy-W(3-hydroxypropyl)-3,3-dimethylbutanamide   386,15   392,489   472,342     26   pentan-3-ol   313,15   322,204   369,393     27   oct-1-en-3-ol   341,15   349,948   367,998     28   2,2-4-rifimorehtanol   302,15   369,64   366,387     29   2,3-4-rimethylpentan-1-ol   314,15   322,25   316,17     31   2-methylbutan-2-ol   314,15   322,25   316,17     32   3,3-dimethylbutan-1-ol   302,15   306,488   311,749     33   2-ethylbutan-1-ol   350,15   332,904   347,934     34   2-ethylbutan-1-ol   350,15   332,904   347,934     35   2,2-4-rifimethylpentan-1-ol   350,15   333,407   325,531     36   3-methylheptan-3-ol   327,15   330,342   307,342     37   tetradecan-1-ol   377,15   364,265   369,771     38   5-methylpentan-1-ol   389,15   397,031   404,333     40   4-methylpentan-1-ol   389,15   397,031   404,333     41   propan-2-ol"   284,817   315,046   305,322     42   butan-1-ol"   308,817   315,798   307,993     44   3-methylbutan-1-ol   390,372   325,364   309,384     47   propan-2-ol"   340,393   340,994   341,994     48   2-tetrahydrotrumylmethanol"   347,393   349,948   341,434     49   40   40   40   40   40   40   40  |     |   |                              |                     |           |
| 18   |     |   |                              |                     |           |
| 19   |     |   |                              |                     |           |
| Deptan=1-ol   332.15   33.5.21   333.879   21   Deptan=1-ol   346.15   341.512   332.95   22   Dexan=2-ol   314.15   377.27   321.81   31.81   32.272   321.81   32.37   32.   |     |   |                              |                     |           |
| 21   |     | ,   |                              |                     |           |
| 22   |     | *   |                              |                     |           |
| 23   |     | 1   |                              |                     |           |
| 24   |     |   |                              |                     |           |
| 25   |     | 1-methoxypropan-2-ol  | 306.15                       | 318.024             | 333.533   |
| 26   pentan-3-ol   313.15   322.204   305.993  |     | octan-1-ol  | 354.15                       | 350.79              | 346.454   |
| 27   |     | (2r)-2,4-dihydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutanamide | 386.15                       | 392.489             |           |
| 28   |     | pentan-3-ol   | 313.15                       | 322.204             | 305.993   |
| 29   | 27  | oct-1-en-3-ol   | 341.15                       | 349.948             | 367.998   |
| 30   | 28  | 2,2,2-trifluoroethanol  | 302.15                       | 296.24              | 306.357   |
| 31   2-methylbutan-1-ol   293.15   296.24   288.576   32   3.3-dimethylbutan-1-ol   302.15   305.488   311.749   33   2-ethylbutan-1-ol   301.15   334.407   325.531   34   2-ethylbutan-1-ol   350.15   334.407   325.531   34   2-ethylbetan-1-ol   350.15   335.94   347.905   352.24.4-trimethylpetan-1-ol   377.15   336.342   307.242   37   tetradecan-1-ol   418.15   406.279   416.163   38   5-methylheptan-3-ol   377.15   349.106   332.81   39   8-methylnonan-1-ol   377.15   344.265   349.106   332.81   41   propan-2-ol"   284.817   293.617   278.532   41   propan-2-ol"   284.817   293.617   278.532   42   butan-1-ol"   309.817   313.798   297.732   43   pentan-1-ol"   330.372   323.046   308.322   44   3-methylbutan-1-ol"   340.928   349.948   311.449   45   cyclohexanol"   340.928   349.948   311.449   46   octan-1-ol"   363.706   350.79   346.454   47   prop-2-en-1-ol"   295.372   304.55   326.94   48   2-tetrahydrofuranylmethanol"   377.039   352.944   389.948   311.449   48   2-tetrahydrofuranylmethanol"   377.36   349.948   34   | 29  | 2,3,4-trimethylpentan-1-ol                                    | 333.15                       | 351.918             | 330.423   |
| 32. 3.3-dimethylbutan-1-ol 30.1.5 30.488 311.749 33  | 30  | 4-methylpentan-2-ol   | 314.15                       | 322.251             | 316.174   |
| 33   | 31  | 2-methylbutan-2-ol  | 293.15                       | 296.24              | 288.576   |
| 34   | 32  | 3,3-dimethylbutan-1-ol  | 302.15                       | 305.488             | 311.749   |
| 35   | 33  | 2-ethylbutan-1-ol   | 330.15                       | 334.407             | 325.531   |
| 36   3-methylheptan-3-ol   327,15   336,342   307,242   161,63   38   161,64   161   | 34  | 2-ethylhexan-1-ol   | 350.15                       | 352.904             | 347.905   |
| 37   | 35  | 2,2,4-trimethylpentan-1-ol                                    | 333.15                       | 331.32              | 325.312   |
| 38         5-methylheptan-3-ol         327.15         349.106         332.281           39         8-methylnonan-1-ol         377.15         364.265         369.771           40         tridecan-1-ol         389.15         397.031         404.323           41         propan-2-ol"         284.817         293.617         278.532           42         butan-1-ol"         309.817         313.798         297.732           43         pentan-1-ol"         303.372         323.046         308.322           44         3-methylbutan-1-ol"         324.817         318.024         317.046           45         cyclohexanol"         340.928         349.948         311.449           46         octan-1-ol"         363.706         350.79         346.454           47         prop-2-en-1-ol"         295.372         304.55         326.194           48         2-tetrahydrofuranylmethanol"         383.15         361.058         378.618           50         5-methylheptan-1-ol"         383.15         361.058         378.618           51         ethylene glycol         392.594         389.86         375.36           52         2-(2-hydroxyethoxy)ethoxylethoxylethoxylethoxylethoxylethoxylethoxylethoxylethoxylethoxyle   | 36  | 3-methylheptan-3-ol   | 327.15                       | 336.342             | 307.242   |
| 39   8-methylnonan-1-ol   377.15   364.265   369.771   40   tridecan-1-ol   389.15   397.031   404.323   41   propan-2-ol"   284.817   293.617   278.532   42   butan-1-ol"   309.817   313.798   297.732   43   pentan-1-ol"   39.817   313.798   297.732   43   pentan-1-ol"   324.817   318.024   317.046   45   cyclohexanol"   324.817   318.024   317.046   45   cyclohexanol"   349.928   349.948   311.449   46   octan-1-ol"   363.706   350.79   346.454   47   prop-2-en-1-ol"   363.706   350.79   346.544   47   prop-2-en-1-ol"   347.039   352.904   352.845   361.058   378.618   50   5-methylheptan-1-ol"   347.039   352.904   352.845   349.948   408.592   349.948   408.592   349.948   408.592   349.948   408.592   349.948    | 37  | tetradecan-1-ol   | 418.15                       | 406.279             | 416.163   |
| 40   | 38  | 5-methylheptan-3-ol   | 327.15                       | 349.106             | 332.281   |
| 1  | 39  | 8-methylnonan-1-ol  | 377.15                       | 364.265             | 369.771   |
| 1  | 40  | tridecan-1-ol   | 389.15                       | 397.031             | 404.323   |
| 330.372   323.046   308.322   344   3-methylbutan-1-ol"   324.817   318.024   317.046   349.928   349.948   311.449   349.928   349.948   311.449   349.928   349.948   311.449   349.928   349.948   311.449   363.706   350.79   346.454   349.948   | 41  | propan-2-ol <sup>a</sup>                                      | 284.817                      | 293.617             | 278.532   |
| 3-methylbutan-1-olf"   324.817   318.024   317.046   | 42  | butan-1-ol <sup>a</sup>                                       | 309.817                      | 313.798             | 297.732   |
| 45   | 43  | pentan-1-ol <sup>a</sup>                                      | 330.372                      | 323.046             | 308.322   |
| 46   | 44  | 3-methylbutan-1-ol <sup>a</sup>                               | 324.817                      | 318.024             |           |
| 46         octan-1-ol <sup>a</sup> 363,706         350,79         346,454           47         prop-2-en-1-ol <sup>a</sup> 295,372         304,55         326,194           48         2-tetrahydrofuranylmethanol <sup>a</sup> 387,039         352,904         352,845           49         (1R)-1-(2-furyl)ethanol <sup>a</sup> 383,15         361,058         378,618           50         5-methylheptan-1-ol <sup>a</sup> 392,594         389,86         375,36           Class: Polyhydric Alcohols           51         ethylene glycol         392,594         389,86         375,36           52         2-(2-hydroxyethoxy)ethanol         411,483         411,722         407,13           53         2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethanol         477,594         438,116         478,926           54         2-[2-[2-(2-hydroxyethoxy)ethoxy]ethox   | 45  | cyclohexanol <sup>a</sup>                                     | 340.928                      | 349.948             | 311.449   |
| 48         2-tetrahydrofuranylmethanol <sup>a</sup> 347.039         352.904         352.845           49         (1R)-1-(2-furyl)ethanol <sup>a</sup> 383.15         361.058         378.618           50         5-methylheptan-1-ol <sup>a</sup> 349.948         408.592           Class: Polyhydric Alcohols           51         ethylene glycol         392.594         389.86         375.36           52         2-(2-hydroxyethoxy)ethanol         411.483         411.722         407.13           53         2-[2-(2-hydroxyethoxy)ethoxy]ethanol         435.928         423.681         445.617           54         2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethanol         477.594         438.116         478.926           55         propane-1,2-diol         377.594         380.062         373.765           56         3-(3-hydroxypropoxy)propany)propanylpro  | 46  | octan-1-ol <sup>a</sup>                                       |                              | 350.79              | 346.454   |
| 49   | 47  | prop-2-en-1-ol <sup>a</sup>                                   | 295.372                      | 304.55              | 326.194   |
| Solution   | 48  | 2-tetrahydrofuranylmethanol <sup>a</sup>                      | 347.039                      | 352.904             | 352.845   |
| Class: Polyhydric Alcohols  51 ethylene glycol 392.594 389.86 375.36 52 2-(2-hydroxyethoxy)ethanol 411.483 411.722 407.13 53 2-[2-(2-hydroxyethoxy)ethoxy]ethanol 435.928 423.681 445.617 54 2-[2-[2-(2-hydroxyethoxy)ethoxy]ethanol 477.594 438.116 478.926 55 propane-1,2-diol 377.594 380.062 373.765 56 3-(3-hydroxypropoxy)propan-1-ol 397.039 420.52 422.148 57 2-[2-(2-hydroxypropoxy)propany]propan-1-ol 416.483 409.9 412.671 58 glycerol 433.15 401.138 424.783 59 butane-1,3-diol 382.039 380.919 392.755 60 butane-1,4-diol 394.261 404.435 394.196 61 pentane-1,5-diol 372.15 380.062 369.324 62 propane-1,1-diol 372.15 380.062 369.324 63 propane-1,3-diol 352.15 402.925 382.459 64 butane-2,3-diol 358.15 388.364 366.991 66 (E)-but-2-ene-1,4-diol 401.15 404.435 377.609 67 but-2-yne-1,4-diol 425.15 404.435 377.609 68 hexane-2,5-diol 420.15 414.388 417.903 69 hexane-2,5-diol 374.15 374.379 395.676   | 49  | (1R)-1- $(2$ -furyl)ethanol <sup>a</sup>                      | 383.15                       | 361.058             | 378.618   |
| 51       ethylene glycol       392.594       389.86       375.36         52       2-(2-hydroxyethoxy)ethonol       411.483       411.722       407.13         53       2-[2-(2-hydroxyethoxy)ethoxy]ethonol       435.928       423.681       445.617         54       2-[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethonol       477.594       438.116       478.926         55       propane-1,2-diol       377.594       380.062       373.765         56       3-(3-hydroxypropoxy)propan-1-ol       397.039       420.52       422.148         57       2-[2-(2-hydroxypropoxy)propany]propan-1-ol       416.483       409.9       412.671         58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,3-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-2,3-diol       366.15       401.138       385.339         65 </td <td>50</td> <td>5-methylheptan-1-ol<sup>a</sup></td> <td></td> <td>349.948</td> <td>408.592</td>  | 50  | 5-methylheptan-1-ol <sup>a</sup>                              |                              | 349.948             | 408.592   |
| 51       ethylene glycol       392.594       389.86       375.36         52       2-(2-hydroxyethoxy)ethonol       411.483       411.722       407.13         53       2-[2-(2-hydroxyethoxy)ethoxy]ethonol       435.928       423.681       445.617         54       2-[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethonol       477.594       438.116       478.926         55       propane-1,2-diol       377.594       380.062       373.765         56       3-(3-hydroxypropoxy)propan-1-ol       397.039       420.52       422.148         57       2-[2-(2-hydroxypropoxy)propany]propan-1-ol       416.483       409.9       412.671         58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,3-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-2,3-diol       366.15       401.138       385.339         65 </td <td></td> <td>Class: Polyhydric Alcohols</td> <td>3</td> <td></td> <td></td>  |     | Class: Polyhydric Alcohols                                    | 3                            |                     |           |
| 52       2-(2-hydroxyethoxy)ethoxy)ethoxy]ethanol       411.483       411.722       407.13         53       2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethanol       435.928       423.681       445.617         54       2-[2-(2-hydroxyethoxy)ethoxy]etho   | 51  |   |                              | 200.07              | 275.27    |
| 53       2-[2-(2-hydroxyethoxy)ethoxy]ethonol       435.928       423.681       445.617         54       2-[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethonol       477.594       438.116       478.926         55       propane-1,2-diol       377.594       380.062       373.765         56       3-(3-hydroxypropoxy)propan-1-ol       397.039       420.52       422.148         57       2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol       416.483       409.9       412.671         58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       387.609         68   |     |   |                              |                     |           |
| 54       2-[2-[2-(2-hydroxyethoxy)ethoxy]ethox   |     |   |                              |                     |           |
| 55       propane-1,2-diol       377.594       380.062       373.765         56       3-(3-hydroxypropoxy)propan-1-ol       397.039       420.52       422.148         57       2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol       416.483       409.9       412.671         58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       387.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 56       3-(3-hydroxypropoxy)propan-1-ol       397.039       420.52       422.148         57       2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol       416.483       409.9       412.671         58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       387.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 57       2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol       416.483       409.9       412.671         58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       337.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 58       glycerol       433.15       401.138       424.783         59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676   |     |   |                              |                     |           |
| 59       butane-1,3-diol       382.039       380.919       392.755         60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 60       butane-1,4-diol       394.261       404.435       394.196         61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676   |     | · ·   |                              |                     |           |
| 61       pentane-1,5-diol       402.594       411.722       406.614         62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 62       propane-1,1-diol       372.15       380.062       369.324         63       propane-1,3-diol       352.15       402.925       382.459         64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 63 propane-1,3-diol 352.15 402.925 382.459 64 butane-1,2-diol 366.15 401.138 385.339 65 butane-2,3-diol 358.15 388.364 366.991 66 (E)-but-2-ene-1,4-diol 401.15 404.435 383.484 67 but-2-yne-1,4-diol 425.15 404.435 377.609 68 hexane-1,6-diol 420.15 414.388 417.903 69 hexane-2,5-diol 374.15 374.379 395.676   |     | * · · · ·   |                              |                     |           |
| 64       butane-1,2-diol       366.15       401.138       385.339         65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     | 1 1 .   |                              |                     |           |
| 65       butane-2,3-diol       358.15       388.364       366.991         66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 66       (E)-but-2-ene-1,4-diol       401.15       404.435       383.484         67       but-2-yne-1,4-diol       425.15       404.435       377.609         68       hexane-1,6-diol       420.15       414.388       417.903         69       hexane-2,5-diol       374.15       374.379       395.676  |     |   |                              |                     |           |
| 67 but-2-yne-1,4-diol 425.15 404.435 <b>377.609</b> 68 hexane-1,6-diol 420.15 414.388 <b>417.903</b> 69 hexane-2,5-diol 374.15 374.379 <b>395.676</b>  |     |   |                              |                     |           |
| 68 hexane-1,6-diol 420.15 414.388 <b>417.903</b><br>69 hexane-2,5-diol 374.15 374.379 <b>395.676</b>   |     | (E)-but-2-ene-1,4-diol  |                              | 404.435             | 383.484   |
| 69 hexane-2,5-diol 374.15 374.379 <b>395.676</b>   |     | but-2-yne-1,4-diol  |                              | 404.435             | 377.609   |
|  | 68  | hexane-1,6-diol   | 420.15                       | 414.388             | 417.903   |
| 70 2.2 disthylanopage 1.2 disl 300.15 410.01 202.10W   | 69  |   | 374.15                       | 374.379             | 395.676   |
| 70 2,2-diethylpropane-1,5-diol 383.197   | 70  | 2,2-diethylpropane-1,3-diol                                   | 380.15                       | 419.21              | 383.197   |

|     |  | _,                           | $T_{\rm f}({\rm predicted})$ (K) |        |
|-----|--|------------------------------|----------------------------------|--------|
| no. | iupac/cas name   | $T_{\rm f}({\rm exptl})$ (K) | MLR                              | ANN    |
| 71  | 2,5-dimethylhex-3-yne-2,5-diol                                     | 347.05                       | 344.495                          | 342.3  |
| 72  | benzoic acid [4-[(oxo-phenylmethoxy)methyl]cyclohexyl]methyl ester | 434.15                       | 471.191                          | 445.3  |
| 73  | [4-(hydroxymethyl)phenyl]methanol                                  | 460.95                       | 417.78                           | 455.09 |
| 74  | 2-butyl-2-ethylpropane-1,3-diol                                    | 386.15                       | 430.521                          | 398.38 |
| 75  | 3,6-dimethyloct-4-yne-3,6-diol                                     | 382.15                       | 395.317                          | 383.74 |
| 76  | 2-ethyl-2-(hydroxymethyl)propane-1,3-diol                          | 445.15                       | 419.21                           | 430    |
| 77  | 2,2-bis(hydroxymethyl)propane-1,3-diol                             | 513.15                       | 419.21                           | 437.6  |
| 78  | (2R,3R,4R,5S)-hexane-1,2,3,4,5,6-hexol                             | 422.05                       | 428.185                          | 420.7  |
| 79  | 2-(hydroxymethyl)-2-methylpropane-1,3-diol                         | 433.15                       | 406.717                          | 444.3  |
| 80  | 2,2-dimethylpropane-1,3-diol <sup>a</sup>                          | 424.817                      | 392.84                           | 408.59 |
| 81  | 2-methylpentane-2,4-diol <sup>a</sup>                              | 374.817                      | 355.86                           | 339.10 |
| 82  | (2S)-butane-1,2,4-triol <sup>a</sup>                               | 385.15                       | 406.488                          | 427.45 |
| 83  | 2,3-dimethylbutane-2,3-diol <sup>a</sup>                           | 350.15                       | 388.935                          | 328.3  |
| 84  | 2-ethylhexane-1,3-diol <sup>a</sup>                                | 409.15                       | 428.496                          | 400.47 |
| 85  | 2-(2-hydroxyethylthio)ethanol <sup>a</sup>                         | 433.15                       | 411.722                          | 424.95 |
| 86  | hexane-1,2,6-triol <sup>a</sup>                                    | 471.15                       | 414.417                          | 463.7  |
|     | Class: Hydrocarbons  |                              |                                  |        |
| 87  | pentane  | 224.15                       | 240.353                          | 244.72 |
| 88  | hexane   | 250.15                       | 255.318                          | 258.67 |
| 89  | heptanes   | 272.15                       | 270.283                          | 275.4  |
| 90  | octane   | 289.15                       | 285.248                          | 289.98 |
| 91  | nonane   | 304.15                       | 300.212                          | 306.75 |
| 92  | decane   | 319.15                       | 315.177                          | 321.13 |
| 93  | dodecane   | 344.15                       | 345.107                          | 351.05 |
| 94  | cyclohexane  | 255.15                       | 257.885                          | 257.71 |
| 95  | cyclohexene  | 243.15                       | 257.885                          | 247.57 |
| 96  | benzene  | 262.15                       | 257.885                          | 228.33 |
| 97  | methylbenzene  | 280.15                       | 269.673                          | 284.39 |
| 98  | 1,2-dimethylbenzene  | 305.15                       | 281.965                          | 334.50 |
| 99  | 1,4-dimethylbenzene  | 300.15                       | 281.461                          | 328.90 |
| 100 | 1,3,5-trimethylbenzene   | 317.15                       | 293.249                          | 355.19 |
| 101 | isopropylbenzene   | 319.15                       | 296.93                           | 349.88 |
| 102 | tridecane  | 352.15                       | 360.072                          | 366.40 |
| 103 | tetradecane  | 372.15                       | 375.037                          | 378.9  |
| 104 | hexadecane   | 408.15                       | 404.967                          | 404.40 |
| 105 | heptadecane  | 421.15                       | 419.932                          | 417.10 |
| 106 | nonadecane   | 441.15                       | 449.862                          | 438.09 |
| 107 | isopentane   | 222.15                       | 236.038                          | 235.87 |
| 108 | isohexane  | 250.15                       | 251.003                          | 248.60 |
| 109 | 3-methylpentane  | 241.15                       | 252.141                          | 247.18 |
| 110 | 2,3-dimethylbutane   | 244.15                       | 247.192                          | 241.40 |
| 111 | buta-1,3-diene   | 197.05                       | 285.775                          | 313.61 |
| 112 | but-2-ene  | 199.85                       | 225.388                          | 213.15 |
| 113 | (z)-but-2-ene  | 200.15                       | 225.388                          | 213.1  |
| 114 | but-1-ene  | 193.15                       | 225.388                          | 230.50 |
| 115 | 2-methylprop-1-ene   | 157.15                       | 219.936                          | 257.35 |
| 116 | (Z)-pent-2-ene   | 255.15                       | 240.353                          | 211.27 |
| 117 | pent-1-ene   | 222.15                       | 240.353                          | 239.40 |
| 118 | dec-1-ene  | 320.15                       | 315.177                          | 307.97 |
| 119 | hept-1-ene   | 264.15                       | 270.283                          | 267.4  |
| 120 | cyclooctane  | 301.15                       | 287.815                          | 292.72 |
| 121 | cyclopenta-1,3-diene   | 273.15                       | 242.92                           | 229.40 |
| 122 | cyclopentane   | 236.15                       | 242.92                           | 242.60 |
| 123 | cyclopentene   | 243.15                       | 242.92                           | 235.4  |
| 124 | 2-methylheptane  | 277.15                       | 280.933                          | 277.2  |
| 125 | 4-vinylcyclohexene   | 294.15                       | 285.775                          | 302.94 |
| 126 | 4-methylpent-1-yne   | 269.15                       | 251.003                          | 267.13 |
| 127 | ethylbenzene <sup>a</sup>  | 295.15                       | 285.775                          | 300.50 |
| 128 | undecane <sup>a</sup>  | 335.15                       | 330.142                          | 337.4  |
| 129 | pentadecane <sup>a</sup>   | 405.15                       | 390.002                          | 393.18 |
| 130 | octadecane <sup>a</sup>  | 439.15                       | 434.897                          | 426.90 |
| 131 | tricosane <sup>a</sup>   | 386.15                       | 509.721                          | 470.08 |
| 132 | 2,2-dimethylbutane <sup>a</sup>                                    | 225.15                       | 244.736                          | 223.05 |
| 133 | 2-methylhexane <sup>a</sup>  | 270.15                       | 265.968                          | 263.38 |
| 134 | but-2-yne <sup>a</sup>   | 260.15                       | 225.388                          | 206.81 |
| 135 | 2,4,4-trimethylpent-1-ene <sup>a</sup>                             | 267.15                       | 270.351                          | 262.58 |
| 136 | 2,3,4-trimethylpent-2-ene <sup>a</sup>                             | 275.15                       | 274.449                          | 284.7  |
|     | Class: Ether   |                              |                                  |        |
| 137 | methoxymethane   | 232.039                      | 228.675                          | 262.6  |
| 138 | ethoxyethane   | 233.15                       | 258.72                           | 237.9  |
|     | 2-methoxy-2-methylpropane  | 238.706                      | 263.12                           | 254.25 |
| 139 | 2-memoxy-2-memyipiopane  | 230.700                      |                                  |        |

Table 4. Continued

|             |   |                              | $T_{\rm f}$ (predicted) (K) |                  |
|-------------|---|------------------------------|-----------------------------|------------------|
| no.         | iupac/cas name  | $T_{\rm f}({\rm exptl})$ (K) | MLR                         | ANN              |
| 141         | 1-butoxybutane  | 304.261                      | 318.811                     | 291.17           |
| 142         | 1-pentoxypentane  | 330.372                      | 348.856                     | 327.25           |
| 143         | 1-ethenoxybutane  | 263.706                      | 288.765                     | 274.49           |
| 144         | 2-methyloxirane   | 235.928                      | 243.085                     | 242.00           |
| 145         | 2-ethyloxirane  | 260.928                      | 259.25                      | 258.00           |
| 146         | 1,4-dioxane   | 291.483                      | 276.32                      | 298.63           |
| 147         | (2,2-dimethyl-1,3-dioxolan-4-yl)methanol                              | 267.039                      | 310.541                     | 320.87           |
| 148         | 2-methylfuran   | 243.15                       | 273.131                     | 280.25           |
| 149         | tetrahydrofuran   | 247.594                      | 261.298                     | 266.44           |
| 150         | tetrahydropyran   | 253.15                       | 276.32                      | 280.53           |
| 151         | methoxybenzene  | 324.817                      | 304.318                     | 321.48           |
| 152         | 1,2-bis(2-methoxyethoxy)ethane  | 386.15                       | 363.879                     | 364.85           |
| 153         | 2-(phenoxymethyl)oxirane  | 388.15                       | 349.916                     | 379.40           |
| 154         | 2-methoxy-2-methylbutane  | 262.15                       | 279.965                     | 278.48           |
| 155         | 2-(2-hydroxyethoxy)ethanol  | 416.15                       | 288.765                     | 407.13           |
| 156         | ethoxyethylene  | 228.15                       | 258.72                      | 259.35           |
| 157         | allyloxybenzene   | 335.15                       | 334.363                     | 336.91           |
| 158         | 2-methoxy-2-methylpropane   | 245.15                       | 263.12                      | 254.25           |
| 159         | phenylmethoxymethylbenzene  | 408.15                       | 410.007                     | 422.25           |
| 160         | 1-chloro-2-(2-chloroethoxy)ethane                                     | 328.15                       | 288.765                     | 328.89           |
| 161         | 1-chloro-2-methoxyethane  | 288.15                       | 258.72                      | 278.95           |
| 162         | 1-[2-(2-butoxyethoxy)ethoxy]butane                                    | 374.15                       | 408.947                     | 373.54           |
| 163         | 3-allyloxyprop-1-ene  | 266.15                       | 288.765                     | 295.1            |
| 164         | 1-chloro-4-(phenoxy)benzene   | 386.15                       | 391.794                     | 415.39           |
| 165         | 1-isopentyloxy-3-methylbutane   | 319.15                       | 340.193                     | 318.73           |
| 166         | 2-(allyloxymethyl)oxirane   | 321.15                       | 304.318                     | 298.39           |
| 167         | chloro-(chloromethoxy)methane   | 292.15                       | 258.72                      | 300.30           |
| 168         | 2-(butoxymethyl)oxirane   | 314.15                       | 319.341                     | 330.12           |
| 169         | 1-chloro-1-(1-chloroethoxy)ethane                                     | 328.15                       | 280.103                     | 305.90           |
| 170         | 1-butoxybutane  | 298.15                       | 318.811                     | 291.17           |
| 171         | 1,2-dimethoxybenzene  | 345.15                       | 332.822                     | 363.19           |
| 172         | 1,2-dimethoxyethane   | 271.15                       | 273.743                     | 292.02           |
| 173         | (3S,3aR,6R,6aR)-3,6-dimethoxy-2,3,3a,5,6,6a-hexahydrofuro[3,2-b]furan | 376.15                       | 362.361                     | 355.04           |
| 174         | phenoxybenzene  | 388.15                       | 379.961                     | 391.75           |
| 175         | 1,3,5-trioxane  | 318.15                       | 276.32                      | 314.38           |
| 176         | ethoxyethylene  | 227.15                       | 258.72                      | 259.3            |
| 177         | 1-hexoxyhexane <sup>a</sup>   | 349.817                      | 378.901                     | 363.13           |
| 178         | ethoxyethylene <sup>a</sup>   | 227.594                      | 258.72                      | 259.3            |
| 179         | 1-ethenoxy-2-methylpropane <sup>a</sup>                               | 263.706                      | 284.434                     | 285.69           |
| 180         | furan <sup>a</sup>  | 237.594                      | 261.297                     | 238.43           |
| 181         | phenoxybenzene <sup>a</sup>   | 388.15                       | 379.961                     | 391.7            |
| 182         | 4-(4-aminophenoxy)aniline <sup>a</sup>                                | 491.15                       | 403.628                     | 464.64           |
| 183         | chloro-methoxymethane <sup>a</sup>                                    | 289.15                       | 243.697                     | 268.98           |
| 184         | 4,7,7-trimethyl-8-oxabicyclo[2.2.2]octane <sup>a</sup>                | 322.15                       | 336.993                     | 322.1            |
| 185         | 1-pentoxypentane <sup>a</sup>   | 330.15                       | 348.856                     | 327.25           |
| 186         | 1-ethenoxypropane <sup>a</sup>  | 247.15                       | 273.743                     | 253.60           |
|             | Class: Amines   |                              |                             |                  |
| 187         | acetamide   | 315.15                       | 278.371                     | 310.27           |
| 188         | 1-(2-pyridyl)ethanone   | 349.15                       | 370.67                      | 389.5            |
| 189         | 2-(bis(2-hydroxyethyl)amino)ethanol                                   | 452.15                       | 390.196                     | 436.3            |
| 190         | prop-2-en-1-amine   | 245.15                       | 290.279                     | 300.60           |
| 191         | 6-methyl-2-pyridinamine   | 376.15                       | 346.839                     | 351.5            |
| 192         | 2-(2-aminoethoxy)ethanol  | 400.15                       | 346.534                     | 385.27           |
| 192         | 2-(2-annioethoxy)ethanor 2-pyridinamine                               | 236.15                       | 341.367                     | 318.2            |
| 193         | aniline   | 343.15                       | 336.39                      | 310.1            |
| 194         | phenylmethanamine   | 345.15                       | 354.535                     | 337.3            |
| 193<br>196  | 3-bromopyridine   | 324.15                       | 314.827                     | 298.99           |
| 190<br>197  | butan-2-amine   | 254.15<br>254.15             | 280.705                     | 283.29           |
| 197         | 2-methylpropan-2-amine  | 235.15                       | 235.866                     | 265.25<br>257.2' |
| 198<br>199  | 2-metnyipropan-2-amine<br>3-chloroaniline                             | 391.15                       | 337.668                     | 352.0°           |
| 200         | 2-chloroaniline   | 391.15<br>371.15             |                             | 365.24           |
| 200<br>201  | 2-chloropyridine  | 371.15                       | 340.514                     |                  |
|             |   |                              | 332.276                     | 306.73           |
| 202         | 2,4,6-trimethylpyridine   | 330.15                       | 343.568                     | 358.22           |
| 203         | 2-pyridinecarbonitrile  | 362.15                       | 366.108                     | 341.90           |
| 204         | 3-pyridinecarbonitrile  | 357.15                       | 365.256                     | 344.99           |
| 205         | 4-pyridinecarbonitrile  | 361.15                       | 365.441                     | 347.08           |
| 206         | 1-cyclohexyl-2-pyrrolidinone  | 418.15                       | 379.197                     | 404.13           |
| 207         | cyclohexanamine   | 300.15                       | 304.905                     | 295.20           |
| 208         | N-pentylpentan-1-amine  | 277.15                       | 382.028                     | 329.30           |
| 209         | 2,6-ditert-butylpyridine  | 345.15                       | 334.552                     | 331.4            |
| 210         | ethane-1,2-diamine  | 330.35                       | 288.59                      | 327.02           |
| 211         | N-cyclohexylcyclohexanamine   | 376.15                       | 380.74                      | 376.2            |
| <b>∠</b> 11 |   |                              |                             | 326.55           |

Table 4. Continued

|     |   |                              | $T_{\rm f}({\rm predicted})$ (K) |         |
|-----|---|------------------------------|----------------------------------|---------|
| no. | iupac/cas name                              | $T_{\rm f}({\rm exptl})$ (K) | MLR                              | ANN     |
| 213 | <i>N</i> -ethylethanamine                   | 245.15                       | 301.613                          | 237.992 |
| 214 | 2-diethylaminoethanol                       | 324.65                       | 348.285                          | 336.194 |
| 215 | diethylcyanamide                            | 342.15                       | 338.401                          | 316.907 |
| 216 | N-(2-aminoethyl)ethane-1,2-diamine          | 363.15                       | 340.071                          | 358.463 |
| 217 | <i>N</i> , <i>N</i> -diethylformamide       | 333.15                       | 336.669                          | 316.305 |
| 218 | 1-(2-hydroxypropylamino)propan-2-ol         | 399.15                       | 343.034                          | 405.999 |
| 219 | n-isopropylpropan-2-amine                   | 266.15                       | 288.95                           | 263.146 |
| 220 | N-methylmethanamine                         | 255.15                       | 265.924                          | 244.246 |
| 221 | N,N-dimethylaniline                         | 336.15                       | 356.04                           | 353.182 |
| 222 | 2-dimethylaminoethanol                      | 313.15                       | 301.33                           | 323.81  |
| 223 | <i>N</i> , <i>N</i> -dimethylformamide      | 330.15                       | 290.798                          | 293.096 |
| 224 | 3,5-dimethylpiperidine                      | 294.65                       | 302.183                          | 303.333 |
| 225 | heptan-2-amine                              | 327.15                       | 321.424                          | 316.324 |
| 226 | heptan-1-amine                              | 317.15                       | 337.285                          | 316.826 |
| 227 | 3-methyl-2-pyridinamine <sup>a</sup>        | 384.15                       | 347.631                          | 371.888 |
| 228 | propan-1-amine <sup>a</sup>                 | 243.15                       | 281.851                          | 259.021 |
| 229 | 2-bromopyridine <sup>a</sup>                | 327.15                       | 318.717                          | 303.486 |
| 230 | butan-1-amine <sup>a</sup>                  | 261.15                       | 295.71                           | 279.44  |
| 231 | 4-chloroaniline <sup>a</sup>                | 461.15                       | 337.778                          | 356.749 |
| 232 | N-allylprop-2-en-1-amine <sup>a</sup>       | 280.15                       | 342.997                          | 286.198 |
| 233 | N-butylbutan-1-amine <sup>a</sup>           | 312.15                       | 354.311                          | 294.626 |
| 234 | 2-(2-hydroxyethylamino)ethanol <sup>a</sup> | 411.15                       | 344.221                          | 405.273 |
| 235 | N,N-dimethylacetamide <sup>a</sup>          | 336.15                       | 298.548                          | 328.412 |
| 236 | 2-aminoethanol <sup>a</sup>                 | 358.15                       | 290.664                          | 351.183 |

<sup>&</sup>lt;sup>a</sup> The solvents belonging to the test set for MLR calculations.

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