

Supporting Information

Liquid Heat Capacity Measurements of the Linear Dicarboxylic Acid Family via Modulated Differential Scanning Calorimetry

*Joseph C. Bloxham, Daniel Hill, Thomas A. Knotts, IV, Neil F. Giles, W. Vincent Wilding**

Department of Chemical Engineering, Brigham Young University, Engineering Building, Rm
330, Provo, Utah 84602, United States

*Corresponding author: Telephone: 801-422-2000, E-mail: vincent_wilding@byu.edu

Linear fits of the data are shown in Figures 2 and 3(?). These are fit to the reported values at each temperature. The model is:

$$y = m x + b$$

Table S1. Linear Fits to Experimental Data in Table 2. Fits Shown in Figures 2 and 3

| Compound | m | b | R ² |
|-----------------------|----------|-------|----------------|
| adipic acid | 0.002314 | 1.452 | 0.9478 |
| pimelic acid | 0.003183 | 1.104 | 1.0 |
| suberic acid | 0.002431 | 1.454 | 0.8750 |
| azelaic acid | .002076 | 1.668 | 0.9594 |
| sebacic acid | 0.002713 | 1.360 | 0.9613 |
| dodecanedioic acid | 0.002860 | 1.383 | 0.9985 |
| tetradecanedioic acid | 0.002220 | 1.784 | 0.9976 |
| dimethyl oxalate | 0.002890 | 0.914 | 0.9525 |

Table S2. Predicted Values Using Ruzicka-Domalski, Ruzicka-Domalski with Constants from Table 3, and the Derivative Method Used to Calculate AAD in Table 4.

| Compound | T/K | Ruzicka-Domalski Values/(J mol ⁻¹ K ⁻¹) | Predicted Updated Predicted Ruzicka-Domalski Values/(J mol ⁻¹ K ⁻¹) | Derivative Method/(J mol ⁻¹ K ⁻¹) |
|--------------|--------|---|--|--|
| adipic acid | 433.09 | 374.0 | 366.9 | 348.4 |
| | 463.07 | 397.0 | 374.1 | 361.8 |
| | 493.04 | 421.2 | 380.2 | 374.6 |
| | 523.01 | 446.8 | 385.3 | 387.3 |
| pimelic acid | 423.09 | 403.8 | 401.5 | 406.3 |
| | 448.07 | 424.3 | 409.7 | 417.3 |
| suberic acid | 423.10 | 441.0 | 438.7 | 465.3 |
| | 448.08 | 463.4 | 448.7 | 479.2 |
| | 473.07 | 486.9 | 458.2 | 491.8 |
| | 513.02 | 526.7 | 472.3 | 509.8 |
| azelaic acid | 393.11 | 450.8 | 461.2 | 482.8 |

| | | | | |
|-----------------------|--------|-------|-------|-------|
| | 433.09 | 487.8 | 480.7 | 508.8 |
| | 473.06 | 527.8 | 499.2 | 531.0 |
| | 513.03 | 571.0 | 516.6 | 550.2 |
| sebacic acid | 413.11 | 505.4 | 507.7 | 504.3 |
| | 453.08 | 546.8 | 529.5 | 537.3 |
| | 493.06 | 591.6 | 550.6 | 566.2 |
| | 533.02 | 639.8 | 570.9 | 592.2 |
| | 572.92 | 691.4 | 590.5 | 617.6 |
| dodecanedioic acid | 423.09 | 589.9 | 587.6 | 573.1 |
| | 448.08 | 619.5 | 604.9 | 595.4 |
| | 473.06 | 650.7 | 622.1 | 616.3 |
| | 523.0 | 717.7 | 656.3 | 654.7 |
| | 572.95 | 791.0 | 690.1 | 691.0 |
| tetradecanedioic acid | 423.10 | 664.3 | 662.1 | 640.3 |
| | 473.06 | 732.6 | 704.0 | 684.5 |
| | 513.02 | 792.4 | 746.6 | 717.0 |
| | 523.02 | 808.1 | 789.7 | 724.8 |
| | 572.97 | 890.6 | 738.0 | 765.9 |

Table S3. Regression Information for Dicarboxylic Acid Prediction Shown in Equation 3

| Compound | T/K | Prediction from eq 3 | AAD (%) |
|--------------|--------|----------------------|---------|
| adipic acid | 433.09 | 357.2 | 0.43% |
| | 463.07 | 369.4 | 0.90% |
| | 493.04 | 381.6 | 0.51% |
| | 523.01 | 393.8 | 1.69% |
| pimelic acid | 423.09 | 392.2 | 1.20% |
| | 448.07 | 403.0 | 1.70% |
| suberic acid | 423.10 | 432.6 | 1.52% |
| | 448.08 | 443.9 | 1.91% |
| | 473.07 | 455.3 | 1.62% |
| | 513.02 | 473.5 | 1.38% |

| | | | |
|-----------------------|--------|-------|-------|
| azelaic acid | 393.11 | 459.7 | 0.27% |
| | 433.09 | 478.8 | 1.78% |
| | 473.06 | 497.9 | 0.95% |
| | 513.03 | 517.0 | 1.22% |
| sebacic acid | 413.11 | 511.8 | 2.13% |
| | 453.08 | 531.8 | 1.77% |
| | 493.06 | 551.8 | 0.35% |
| | 533.02 | 571.8 | 2.65% |
| | 572.92 | 591.8 | 0.30% |
| dodecanedioic acid | 423.09 | 605.8 | 1.59% |
| | 448.08 | 619.4 | 0.55% |
| | 473.06 | 633.0 | 0.57% |
| | 523.0 | 660.2 | 0.09% |
| | 572.95 | 687.4 | 1.03% |
| tetradecanedioic acid | 423.10 | 699.3 | 0.78% |
| | 473.06 | 728.5 | 0.28% |
| | 513.02 | 751.9 | 0.19% |
| | 523.02 | 757.8 | 0.61% |
| | 572.97 | 787.0 | 0.39% |
