DSC Experiments

Equilibrium Calculation for Cappa Mixture

Physical Properties of Mixture:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Compound** | **MW**  **(g mol-1)** | **Enthalpy (kJ mol-1)a** | **Vapor Pressure (atm)** | **Density**  **(g cm-3)** | **Mole Fraction** | **Mass Fraction** |
| Malonic Acid | 104.06 | 141.9 | 6.61E-09 | 1.619 | 0.111 | 0.0715 |
| Succinic Acid | 118.09 | 88.5 | 3.1E-09 | 1.56 | 0.111 | 0.0812 |
| Glutaric Acid | 132.11 | 141.0 | 1.73E-09 | 1.429 | 0.111 | 0.0908 |
| Adipic Acid | 146.14 | 111.0 | 9.7E-10 | 1.36 | 0.111 | 0.1005 |
| Pimelic Acid | 160 | 124.0 | 5.51E-10 | 1.28 | 0.111 | 0.1100 |
| Suberic Acid | 174 | 130.0 | 3.15E-10 | 1.272 | 0.111 | 0.1196 |
| Azelaic Acid | 188 | 146.0 | 1.81E-10 | 1.0287 | 0.111 | 0.1293 |
| Sebacic Acid | 202 | 140.0 | 1.05E-10 | 1.209 | 0.111 | 0.1389 |
| Dodecanoic Acid | 230 | 119.0 | 1.72E-09 | 0.88 | 0.111 | 0.1581 |
| Total | 161.44b |  |  | 1.242c |  |  |

aCappa et al. (2008)

bMole-weighted

cMass-weighted

Pure component saturation concentration calculation:

Saturation Concentration **(mg m-3)** as a function of temperature:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **T (deg C)** | **5** | **20** | **70** | **100** | **120** |
| Malonic Acid | 3.34E-04 | 7.34E-03 | 3.06E+01 | 1.54E+03 | 1.50E+04 |
| Succinic Acid | 9.69E-04 | 6.53E-03 | 1.11E+00 | 1.24E+01 | 5.03E+01 |
| Glutaric Acid | 1.14E-04 | 2.45E-03 | 9.68E+00 | 4.75E+02 | 4.56E+03 |
| Adipic Acid | 1.83E-04 | 2.03E-03 | 1.33E+00 | 2.81E+01 | 1.65E+02 |
| Pimelic Acid | 7.55E-05 | 1.12E-03 | 1.59E+00 | 4.84E+01 | 3.51E+02 |
| Suberic Acid | 3.88E-05 | 6.56E-04 | 1.34E+00 | 4.82E+01 | 3.86E+02 |
| Azelaic Acid | 1.45E-05 | 3.50E-04 | 1.86E+00 | 1.05E+02 | 1.10E+03 |
| Sebacic Acid | 1.09E-05 | 2.31E-04 | 8.56E-01 | 4.08E+01 | 3.86E+02 |
| Dodecanoic Acid | 3.97E-04 | 5.25E-03 | 5.55E+00 | 1.46E+02 | 9.80E+02 |

Pure Component Condensed Mass Fraction:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Liquid Mass**  **(mg)** | **Liquid Vol.**  **(cm3)** | **Mass Concentration (mg m-3)\*** | **Condensed Mass Fraction** |
| Malonic Acid | 0.72 | 4.42E-04 | 8.89E+06 | 0.99 |
| Succinic Acid | 0.81 | 5.20E-04 | 1.01E+07 | 1.00 |
| Glutaric Acid | 0.91 | 6.36E-04 | 1.13E+07 | 0.99 |
| Adipic Acid | 1.00 | 7.39E-04 | 1.25E+07 | 0.99 |
| Pimelic Acid | 1.10 | 8.59E-04 | 1.37E+07 | 0.99 |
| Suberic Acid | 1.20 | 9.41E-04 | 1.49E+07 | 0.99 |
| Azelaic Acid | 1.29 | 1.26E-03 | 1.61E+07 | 0.99 |
| Sebacic Acid | 1.39 | 1.15E-03 | 1.73E+07 | 0.99 |
| Dodecanoic Acid | 1.58 | 1.80E-03 | 1.96E+07 | 0.99 |
| Total | 10.00 | 8.05E-03 | 1.24E+08 | 1.00 |

\*Assume cell volume is approximately 10x larger than liquid volume