

**Table S1: Estimated sub-cooled liquid vapour pressures at 298 K. N\_Vp (Nannoolal vapour pressure), MY\_Vp (Myrdal and Yalkowsky vapour pressure, SIMPOL (SIMPOL vapour pressure), N\_Tb (Nannoolal boiling point), SB\_Tb (Stein and Brown boiling point), Literature (4-dimethylaminobenzaldehyde from Daubert and Danner (Daubert and Danner, 1989), 3-ethoxy-4-hydroxybenzaldehyde, vanillin, and 4-hydroxybenzaldehyde from Yaws (Yaws, 1994). Error bars are +/- 1 standard deviation. This table contains the corresponding information used in Fig. 7**

| Compound                           | N_Vp &<br>N_Tb (Pa) | N_Vp &<br>SB_Tb (Pa) | MY_Vp &<br>N_Tb (Pa) | MY_Vp &<br>SB_Tb (Pa) | SIMPOL (Pa) | Literature (Pa) | Experimental (Pa) |
|------------------------------------|---------------------|----------------------|----------------------|-----------------------|-------------|-----------------|-------------------|
| methyl 4-formylbenzoate            | 8.82E-01            | 1.28E+00             | 1.73E+00             | 2.47E+00              | 1.11E+01    | nan             | 1.07E+00          |
| terephthalaldehyde                 | 6.67E-01            | 2.94E+00             | 1.22E+00             | 5.09E+00              | 1.41E+00    | nan             | 9.43E-01          |
| o-vanillin                         | 2.35E-01            | 4.29E-01             | 2.85E-01             | 5.15E-01              | 2.20E-02    | nan             | 6.44E-01          |
| 2,4-dimethoxy-3-methylbenzaldehyde | 2.69E-01            | 4.73E-01             | 6.85E-01             | 1.16E+00              | 3.95E-02    | nan             | 2.38E-01          |
| 2,3,4-trimethoxybenzaldehyde       | 5.82E-02            | 1.34E-01             | 2.05E-01             | 4.41E-01              | 3.84E-03    | nan             | 1.73E-01          |
| 4-dimethylamino benzaldehyde       | 6.15E+00            | 9.38E+00             | 5.22E+00             | 8.11E+00              | 2.90E-01    | 4.91E-01        | 1.57E-01          |
| 3,4-dimethoxy benzaldehyde         | 7.82E-01            | 1.43E+00             | 1.54E+00             | 2.76E+00              | 1.05E-01    | nan             | 1.38E-01          |
| 3-ethoxy-4-hydroxy benzaldehyde    | 1.64E-01            | 1.94E-01             | 1.76E-01             | 2.09E-01              | 8.29E-03    | 1.39E-03        | 1.31E-01          |
| 3-ethoxy-4-methoxy benzaldehyde    | 5.36E-01            | 6.52E-01             | 8.69E-01             | 1.05E+00              | 3.95E-02    | nan             | 1.14E-01          |
| 3-hydroxy benzaldehyde             | 3.24E+00            | 4.29E+00             | 2.32E+00             | 3.11E+00              | 6.01E-01    | nan             | 9.21E-02          |
| 2,5-dihydroxy benzaldehyde         | 3.53E-02            | 8.87E-02             | 5.83E-02             | 1.40E-01              | 4.61E-03    | nan             | 7.02E-02          |
| vanillin                           | 2.35E-01            | 4.29E-01             | 2.85E-01             | 5.15E-01              | 2.20E-02    | 1.57E-02        | 6.73E-02          |

|                                |          |          |          |          |          |          |          |
|--------------------------------|----------|----------|----------|----------|----------|----------|----------|
| 4-diethylamino<br>benzaldehyde | 2.85E+00 | 2.12E+00 | 1.59E+00 | 1.15E+00 | 4.11E-02 | nan      | 6.49E-02 |
| 2,6-dimethoxy<br>benzaldehyde  | 7.82E-01 | 1.43E+00 | 1.54E+00 | 2.76E+00 | 1.05E-01 | nan      | 4.50E-02 |
| 4-hydroxy<br>benzaldehyde      | 2.70E+00 | 4.26E+00 | 1.94E+00 | 3.11E+00 | 6.01E-01 | 1.51E-02 | 2.78E-02 |
| isovanillin                    | 2.35E-01 | 4.29E-01 | 2.85E-01 | 5.15E-01 | 2.20E-02 | nan      | 2.36E-02 |
| 2-carboxy<br>benzaldehyde      | 1.50E-02 | 2.09E-02 | 6.83E-02 | 9.16E-02 | 9.11E-03 | nan      | 4.96E-03 |

## References

Daubert, T. E. and Danner, R. P.: Physical and thermodynamic properties of pure chemicals: data compilation, Hemisphere Pub. Corp., New York., 1989.

Yaws, C. L.: Handbook of vapor pressure, Gulf Pub. Co., Houston., 1994.