

## Supplemental information for

### Measurement of Henry's law and liquid-phase loss rate constants of peroxypropionic nitric anhydride (PPN) in deionized water and in n-octanol

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**Table S1.** Schedule of experiments: PAN in DI water.

| Internal reference | GC-ECD | $T$<br>(°C) | $V_l$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_l}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|--------------------|--------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| KN 211026          | HP     | 20.0±0.1    | 140±2         | 317±3                             | 2.26±0.04                                  | 0.0532±0.0006                                                                     |
| KN 211028          | HP     | 20.0±0.1    | 140±2         | 532±6                             | 3.80±0.07                                  | 0.0592±0.0010                                                                     |
| AM 211108          | Varian | 20.00±0.01  | 140±2         | 124±1                             | 0.89±0.02                                  | 0.0302±0.0001                                                                     |
| HO 211108          | HP     | 5.0±0.1     | 100±2         | 240±3                             | 2.40±0.05                                  | 0.0190±0.0003                                                                     |
| AM 211116          | Varian | 5.00±0.01   | 50.0±0.4      | 481±5                             | 9.6±0.1                                    | 0.0466±0.0001                                                                     |
| KN 211118          | HP     | 5.0±0.1     | 75.0±0.4      | 541±6                             | 7.21±0.09                                  | 0.0394±0.0003                                                                     |
| KN 211104          | HP     | 5.0±0.1     | 30.0±0.4      | 433±5                             | 14.4±0.2                                   | 0.0639±0.0004                                                                     |
| KN 211116          | HP     | 5.0±0.1     | 100±2         | 481±5                             | 4.81±0.11                                  | 0.0299±0.0002                                                                     |
| KN 211118          | HP     | 20.0±0.1    | 140±2         | 177±2                             | 1.27±0.02                                  | 0.0299±0.0002                                                                     |
| KN 211123          | HP     | 20.0±0.1    | 140±2         | 570±6                             | 4.07±0.07                                  | 0.0654±0.0011                                                                     |
| AM 211123          | Varian | 5.00±0.01   | 75.0±0.4      | 451±5                             | 6.01±0.07                                  | 0.0309±0.0001                                                                     |
| KN 211125          | HP     | 20.0±0.1    | 100±2         | 697±8                             | 6.97±0.16                                  | 0.0899±0.0023                                                                     |

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**Table S2.** Schedule of experiments: PPN in DI water. Experiments were conducted with the Varian GC-ECD.

| Internal reference | $T$<br>(°C) | $V_l$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_l}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|--------------------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| MV 220301          | 20.00±0.01  | 100±2         | 125±15                            | 1.25±0.15                                  | 0.043±0.005                                                                       |
| MV 220308          | 20.00±0.01  | 100±2         | 433±52                            | 4.33±0.53                                  | 0.085±0.002                                                                       |
| MV 220315-1        | 20.00±0.01  | 150±2         | 496±5                             | 3.33±0.06                                  | 0.0706±0.0010                                                                     |
| MV 220315-2        | 20.00±0.01  | 100±2         | 620±7                             | 6.23±0.14                                  | 0.1235±0.0018                                                                     |
| MV 220317-1        | 5.00±0.01   | 150±2         | 118±1                             | 0.79±0.01                                  | 0.01098±0.00004                                                                   |
| MV 220317-2        | 5.00±0.01   | 150±2         | 294±3                             | 1.97±0.03                                  | 0.01818±0.00005                                                                   |
| MV 220322-1        | 5.00±0.01   | 150±2         | 235±3                             | 1.58±0.02                                  | 0.01533±0.00005                                                                   |
| MV 220322-2        | 5.00±0.01   | 150±2         | 353±4                             | 2.37±0.04                                  | 0.01932±0.00005                                                                   |
| MV 220324-1        | 5.00±0.01   | 150±2         | 176±2                             | 1.18±0.02                                  | 0.01357±0.00002                                                                   |

**Table S2 (continued).** Schedule of experiments: PPN in DI water. Experiments were conducted with the

40 Varian GC-ECD.

| Internal<br>reference | $T$<br>(°C) | $V_l$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_l}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|-----------------------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| MV 220324-2           | 12.50±0.01  | 150±2         | 121±1                             | 0.81±0.01                                  | 0.0204±0.00018                                                                    |
| MV 220329-1           | 12.50±0.01  | 150±2         | 243±3                             | 1.62±0.03                                  | 0.0288±0.0001                                                                     |
| MV 220329-2           | 12.50±0.01  | 150±2         | 365±4                             | 2.43±0.04                                  | 0.0373±0.0001                                                                     |
| MV 220331-1           | 12.50±0.01  | 150±2         | 182±2                             | 1.22±0.02                                  | 0.0251±0.0001                                                                     |
| MV 220321-2           | 12.50±0.01  | 150±2         | 304±3                             | 2.03±0.04                                  | 0.0332±0.0002                                                                     |
| MV 220405-1           | 20.00±0.01  | 150±2         | 375±4                             | 2.50±0.04                                  | 0.0665±0.0001                                                                     |
| MV 220405-2           | 8.50±0.01   | 150±2         | 240±3                             | 1.60±0.03                                  | 0.0212±0.0001                                                                     |
| MV 220405-3           | 8.50±0.01   | 150±2         | 481±5                             | 3.20±0.06                                  | 0.0345±0.0001                                                                     |
| MV 220407-1           | 8.50±0.01   | 150±2         | 353±4                             | 2.35±0.04                                  | 0.0285±0.0001                                                                     |
| MV 220407-2           | 8.50±0.01   | 150±2         | 530±6                             | 3.54±0.06                                  | 0.0388±0.0002                                                                     |
| MV 220407-3           | 5.00±0.01   | 150±2         | 408±4                             | 2.72±0.05                                  | 0.0231±0.0001                                                                     |
| HO 220411-1           | 16.00±0.01  | 150±2         | 430±5                             | 2.87±0.05                                  | 0.0567±0.0003                                                                     |
| HO 220411-2           | 16.00±0.01  | 150±2         | 246±3                             | 1.64±0.03                                  | 0.03744±0.00004                                                                   |
| HO 220412-1           | 16.00±0.01  | 150±2         | 213±2                             | 1.42±0.02                                  | 0.03453±0.00005                                                                   |
| HO 220412-3           | 20.00±0.01  | 150±2         | 246±3                             | 1.64±0.03                                  | 0.0487±0.0001                                                                     |
| HO 220414-1           | 16.00±0.01  | 150±2         | 336±4                             | 2.24±0.04                                  | 0.0451±0.0001                                                                     |
| HO 220414-2           | 16.00±0.01  | 150±2         | 580±6                             | 3.87±0.07                                  | 0.0665±0.0001                                                                     |
| KE 220531-1           | 25.00±0.01  | 100.0±0.4     | 312±3                             | 3.12±0.04                                  | 0.1122±0.0006                                                                     |
| KE 220531-2           | 25.00±0.01  | 100.0±0.4     | 125±1                             | 1.25±0.01                                  | 0.0628±0.0001                                                                     |
| KE 220531-3           | 25.00±0.01  | 100.0±0.4     | 281±3                             | 2.81±0.03                                  | 0.1048±0.0006                                                                     |
| KE 220531-4           | 25.00±0.01  | 100.0±0.4     | 344±4                             | 3.44±0.04                                  | 0.125±0.002                                                                       |
| KE 220603-1           | 25.00±0.01  | 100.0±0.4     | 189±2                             | 1.89±0.02                                  | 0.0810±0.0003                                                                     |

**Table S3.** Schedule of experiments: PPN in n-octanol. Experiments were conducted with the Varian GC-

45 ECD.

| Internal<br>reference | $T$<br>(°C) | $V_l$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_l}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|-----------------------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| KE 220607-1c          | 20.00±0.01  | 50.0±0.4      | 277±3                             | 5.54±0.08                                  | 0.00255±0.00004                                                                   |
| KE 220607-1d          | 20.00±0.01  | 50.0±0.4      | 339±4                             | 6.78±0.09                                  | 0.00381±0.00003                                                                   |
| KE 220609-1b          | 20.00±0.01  | 50.0±0.4      | 186±2                             | 3.73±0.05                                  | 0.00242±0.00005                                                                   |
| KE 220609-1c          | 20.00±0.01  | 50.0±0.4      | 373±4                             | 7.46±0.10                                  | 0.00413±0.00002                                                                   |
| KE 220609-1d          | 20.00±0.01  | 50.0±0.4      | 311±3                             | 6.22±0.08                                  | 0.00374±0.00005                                                                   |
| KE 220609-1e          | 20.00±0.01  | 50.0±0.4      | 125±1                             | 2.49±0.03                                  | 0.00221±0.00002                                                                   |
| KE 220609-1f          | 20.00±0.01  | 50.0±0.4      | 100±1                             | 2.00±0.03                                  | 0.0018152±0.0000009                                                               |
| KE 220610-1           | 20.00±0.01  | 50.0±0.4      | 281±3                             | 5.62±0.08                                  | 0.00363±0.00002                                                                   |
| KE 220621-2a          | 20.00±0.01  | 50.0±0.4      | 259±3                             | 5.17±0.07                                  | 0.00317±0.00002                                                                   |
| KE 220621-2b          | 20.00±0.01  | 50.0±0.4      | 401±4                             | 8.02±0.11                                  | 0.004642±0.000009                                                                 |
| KE 220621-2c          | 20.00±0.01  | 50.0±0.4      | 130±1                             | 2.60±0.04                                  | 0.002091±0.000001                                                                 |
| KE 220622-1           | 20.00±0.01  | 50.0±0.4      | 223±2                             | 4.47±0.06                                  | 0.00346±0.00005                                                                   |
| KE 220622-2b          | 5.00±0.01   | 50.0±0.4      | 384±4                             | 7.68±0.10                                  | 0.00152±0.00001                                                                   |
| KE 220622-2c          | 5.00±0.01   | 50.0±0.4      | 118±1                             | 2.37±0.03                                  | 0.000562±0.000001                                                                 |
| KE 220623-1           | 5.00±0.05   | 50.0±0.4      | 177±2                             | 3.54±0.05                                  | 0.0008265±0.0000009                                                               |
| KE 220624-1a          | 5.00±0.05   | 50.0±0.4      | 234±3                             | 4.68±0.06                                  | 0.00144±0.00003                                                                   |
| KE 220624-1b          | 5.00±0.05   | 50.0±0.4      | 321±4                             | 6.42±0.09                                  | 0.00176±0.00004                                                                   |
| KE 220624-1c          | 5.00±0.05   | 50.0±0.4      | 350±4                             | 7.00±0.10                                  | 0.00202±0.00005                                                                   |
| KE 220627-1a          | 25.00±0.01  | 50.0±0.4      | 312±3                             | 6.25±0.09                                  | 0.00533±0.00009                                                                   |
| KE 220627-1b          | 25.00±0.01  | 50.0±0.4      | 125±1                             | 2.50±0.03                                  | 0.00379±0.00003                                                                   |
| KE 220627-1c          | 25.00±0.01  | 50.0±0.4      | 282±3                             | 5.64±0.08                                  | 0.00543±0.00002                                                                   |
| KE 220627-1d          | 25.00±0.01  | 50.0±0.4      | 188±2                             | 3.76±0.05                                  | 0.00439±0.00001                                                                   |
| KE 220627-1e          | 25.00±0.01  | 50.0±0.4      | 345±4                             | 6.89±0.09                                  | 0.005763±0.000005                                                                 |
| KE 220628-1a          | 16.00±0.01  | 50.0±0.4      | 304±3                             | 6.09±0.08                                  | 0.0027±0.0001                                                                     |
| KE 220628-1c          | 16.00±0.01  | 50.0±0.4      | 275±3                             | 5.49±0.07                                  | 0.00263±0.00003                                                                   |
| KE 220628-1d          | 16.00±0.01  | 50.0±0.4      | 183±2                             | 3.67±0.05                                  | 0.00192±0.00003                                                                   |
| KE 220628-1e          | 16.00±0.01  | 50.0±0.4      | 337±4                             | 6.74±0.09                                  | 0.002889±0.000001                                                                 |
| KE 220629-2c          | 5.00±0.01   | 50.0±0.4      | 200±2                             | 4.01±0.05                                  | 0.00095±0.00001                                                                   |

**Table S3 (continued).** Schedule of experiments: PPN in n-octanol. Experiments were conducted with the Varian GC-ECD.

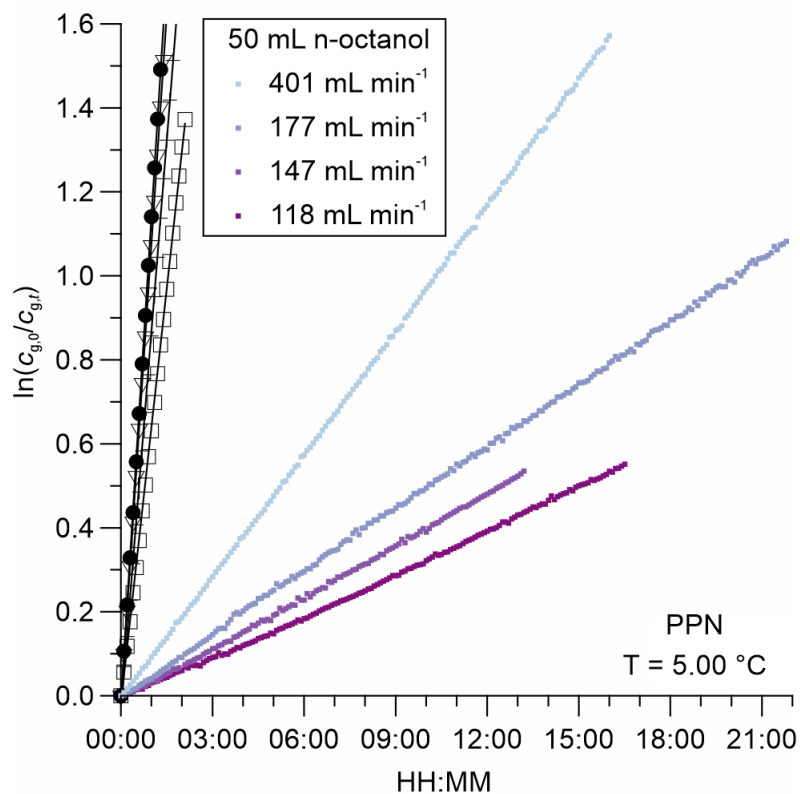
|    | Internal<br>reference | $T$<br>(°C) | $V_I$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_I}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|----|-----------------------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| 50 | KE 220711-1b          | 8.50±0.01   | 50.0±0.4      | 118±1                             | 2.37±0.03                                  | 0.000843±0.000009                                                                 |
|    | KE 220711-1c          | 8.50±0.01   | 50.0±0.4      | 267±3                             | 5.34±0.07                                  | 0.00155±0.00001                                                                   |
|    | KE 220711-1d          | 8.50±0.01   | 50.0±0.4      | 178±2                             | 3.56±0.05                                  | 0.0010546±0.0000009                                                               |
|    | KE 220712-1a          | 8.50±0.01   | 50.0±0.4      | 327±4                             | 6.55±0.09                                  | 0.00197±0.00002                                                                   |
| 55 | KE 220712-1b          | 8.50±0.01   | 50.0±0.4      | 238±3                             | 4.77±0.06                                  | 0.00162±0.00002                                                                   |
|    | KE 220712-1c          | 8.50±0.01   | 50.0±0.4      | 358±4                             | 7.16±0.10                                  | 0.00223±0.00004                                                                   |
|    | KE 220712-2b          | 12.50±0.01  | 50.0±0.4      | 121±1                             | 2.43±0.03                                  | 0.001046±0.000002                                                                 |
|    | KE 220713-1a          | 12.50±0.01  | 50.0±0.4      | 273±3                             | 5.46±0.07                                  | 0.00214±0.00002                                                                   |
|    | KE 220713-1b          | 12.50±0.01  | 50.0±0.4      | 182±2                             | 3.64±0.05                                  | 0.00168±0.00002                                                                   |
|    | KE 220713-1c          | 12.50±0.01  | 50.0±0.4      | 334±4                             | 6.68±0.09                                  | 0.0025±0.0001                                                                     |
| 60 | KE 220713-1d          | 12.50±0.01  | 50.0±0.4      | 152±2                             | 3.03±0.04                                  | 0.00161±0.00008                                                                   |
|    | KE 220713-1e          | 12.50±0.01  | 50.0±0.4      | 243±3                             | 4.86±0.07                                  | 0.00206±0.00007                                                                   |
|    | KE 220713-2           | 5.00±0.01   | 50.0±0.4      | 147±2                             | 2.94±0.04                                  | 0.000682±0.000001                                                                 |
|    | KE 220714-1a          | 5.00±0.01   | 50.0±0.4      | 252±3                             | 5.05±0.07                                  | 0.00127±0.00002                                                                   |
|    | KE 220714-1b          | 5.00±0.01   | 50.0±0.4      | 211±2                             | 4.23±0.06                                  | 0.00105±0.00004                                                                   |
| 65 | KE 220714-1c          | 5.00±0.01   | 50.0±0.4      | 382±4                             | 7.64±0.10                                  | 0.00181±0.00003                                                                   |
|    | KE 220714-1d          | 5.00±0.01   | 50.0±0.4      | 265±3                             | 5.29±0.07                                  | 0.00129±0.00003                                                                   |
|    | KE 220714-1e          | 5.00±0.01   | 50.0±0.4      | 306±3                             | 6.12±0.08                                  | 0.00167±0.00006                                                                   |
|    | KE 220718-1b          | 5.00±0.01   | 50.0±0.4      | 354±4                             | 7.09±0.10                                  | 0.00122±0.00003                                                                   |
|    | KE 220718-1c          | 5.00±0.01   | 50.0±0.4      | 331±4                             | 6.62±0.09                                  | 0.00142±0.00001                                                                   |
|    | KE 220718-1d          | 5.00±0.01   | 50.0±0.4      | 401±4                             | 8.02±0.11                                  | 0.001641±0.000001                                                                 |
| 70 | KE 220719-1a          | 5.00±0.01   | 50.0±0.4      | 318±3                             | 6.36±0.09                                  | 0.00167±0.00002                                                                   |
|    | KE 220719-1b          | 5.00±0.01   | 50.0±0.4      | 365±4                             | 7.30±0.10                                  | 0.00195±0.00004                                                                   |
|    | KE 220719-1c          | 5.00±0.01   | 50.0±0.4      | 413±5                             | 8.26±0.11                                  | 0.00206±0.00006                                                                   |
|    | KE 220719-2           | 5.00±0.01   | 100.0±0.6     | 94±1                              | 0.94±0.01                                  | 0.000285±0.000001                                                                 |
|    | KE 220720-1a          | 5.00±0.01   | 100.0±0.6     | 176±2                             | 1.76±0.02                                  | 0.00062±0.00001                                                                   |
|    | KE 220720-1b          | 5.00±0.01   | 100.0±0.6     | 129±1                             | 1.29±0.02                                  | 0.000466±0.000007                                                                 |
| 75 | KE 220720-1c          | 5.00±0.01   | 100.0±0.6     | 188±2                             | 1.88±0.02                                  | 0.000667±0.000008                                                                 |

**Table S3 (continued).** Schedule of experiments: PPN in n-octanol. Experiments were conducted with the Varian GC-ECD.

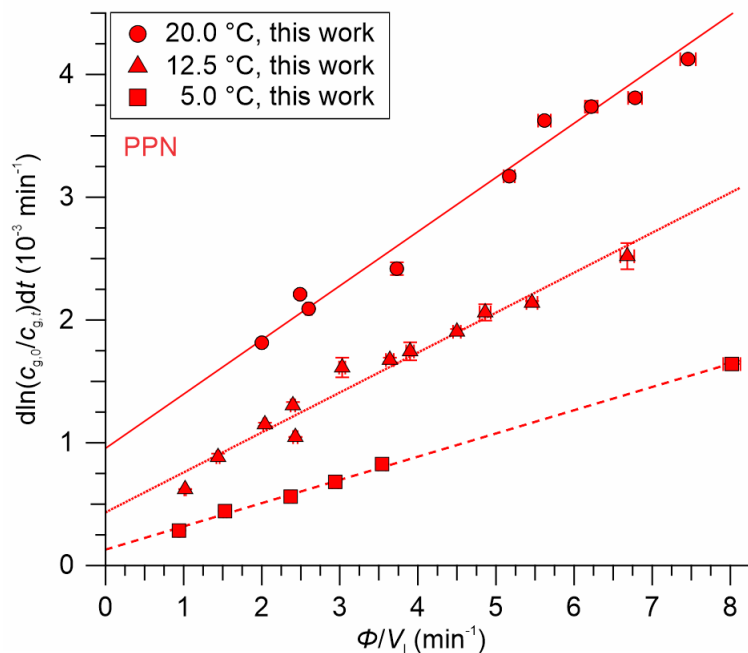
|    | Internal<br>reference | $T$<br>(°C) | $V_l$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_l}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|----|-----------------------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| 80 | KE 220720-1d          | 5.00±0.05   | 100.0±0.6     | 153±2                             | 1.53±0.02                                  | 0.000444±0.000001                                                                 |
|    | KE 220721-1b          | 16.00±0.01  | 50.0±0.4      | 257±3                             | 5.14±0.07                                  | 0.00235±0.00004                                                                   |
|    | KE 220721-1c          | 16.00±0.01  | 50.0±0.4      | 153±2                             | 3.06±0.04                                  | 0.001639±0.000007                                                                 |
|    | KE 220721-1d          | 16.00±0.01  | 50.0±0.4      | 221±2                             | 4.42±0.06                                  | 0.00219±0.00002                                                                   |
|    | KE 220725-1a          | 20.00±0.01  | 100.0±0.4     | 148±2                             | 1.48±0.02                                  | 0.00140±0.00006                                                                   |
| 85 | KE 220725-1b          | 20.00±0.01  | 100.0±0.4     | 432±5                             | 4.32±0.05                                  | 0.00372±0.00009                                                                   |
|    | KE 220725-1c          | 20.00±0.01  | 100.0±0.4     | 99±1                              | 0.99±0.01                                  | 0.00149±0.00003                                                                   |
|    | KE 220725-1d          | 20.00±0.01  | 100.0±0.4     | 185±2                             | 1.85±0.02                                  | 0.00206±0.00001                                                                   |
|    | KE 220725-1e          | 20.00±0.01  | 100.0±0.4     | 463±5                             | 4.63±0.05                                  | 0.00325±0.00003                                                                   |
|    | KE 220725-1f          | 20.00±0.01  | 100.0±0.4     | 111±1                             | 1.11±0.01                                  | 0.001492±0.000001                                                                 |
|    | KE 220726-1a          | 25.00±0.01  | 100.0±0.4     | 150±2                             | 1.50±0.02                                  | 0.00350±0.00009                                                                   |
|    | KE 220726-1b          | 25.00±0.01  | 100.0±0.4     | 100±1                             | 1.00±0.01                                  | 0.00307±0.00007                                                                   |
| 90 | KE 220726-1c          | 25.00±0.01  | 100.0±0.4     | 451±5                             | 4.51±0.05                                  | 0.0050±0.0001                                                                     |
|    | KE 220726-1d          | 25.00±0.01  | 100.0±0.4     | 201±2                             | 2.01±0.02                                  | 0.0033±0.0001                                                                     |
|    | KE 220726-1e          | 25.00±0.01  | 100.0±0.4     | 502±6                             | 5.02±0.06                                  | 0.00513±0.00006                                                                   |
|    | KE 220726-2           | 12.50±0.01  | 100.0±0.4     | 102±1                             | 1.02±0.01                                  | 0.000622±0.000002                                                                 |
|    | KE 220727-1a          | 12.50±0.01  | 100.0±0.4     | 204±2                             | 2.04±0.02                                  | 0.00115±0.00001                                                                   |
|    | KE 220727-1b          | 12.50±0.01  | 100.0±0.4     | 450±5                             | 4.50±0.05                                  | 0.00190±0.00002                                                                   |
| 95 | KE 220727-1c          | 12.50±0.01  | 100.0±0.4     | 144±2                             | 1.44±0.02                                  | 0.00088±0.00003                                                                   |
|    | KE 220727-1d          | 12.50±0.01  | 100.0±0.4     | 390±4                             | 3.90±0.05                                  | 0.00174±0.00007                                                                   |
|    | KE 220727-1e          | 12.50±0.01  | 100.0±0.4     | 240±3                             | 2.40±0.03                                  | 0.00131±0.00003                                                                   |
|    | KE 220727-2           | 8.50±0.01   | 100.0±0.4     | 101±1                             | 1.01±0.01                                  | 0.000438±0.000001                                                                 |
|    | KE 220728-1a          | 8.50±0.01   | 100.0±0.4     | 296±3                             | 2.96±0.03                                  | 0.00118±0.00004                                                                   |

100 **Table S4.** Schedule of experiments: PPN in n-octanol containing  $\sim(0.6\pm0.2)$  mM of  $\alpha$ -tocopherol.  
Experiments were conducted with the Varian GC-ECD.

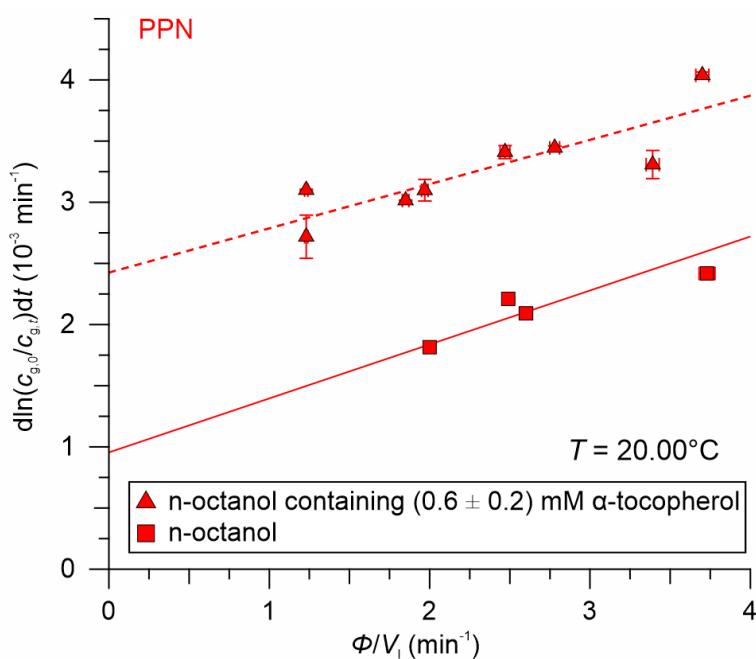
|     | Internal<br>reference | $T$<br>(°C) | $V_l$<br>(mL) | $\Phi$<br>(mL min <sup>-1</sup> ) | $\frac{\Phi}{V_l}$<br>(min <sup>-1</sup> ) | $\frac{d}{dt} \ln \left( \frac{c_{g,0}}{c_{g,t}} \right)$<br>(min <sup>-1</sup> ) |
|-----|-----------------------|-------------|---------------|-----------------------------------|--------------------------------------------|-----------------------------------------------------------------------------------|
| 105 | KE 220809-1b          | 20.00±0.01  | 100.0±0.4     | 123±1                             | 1.23±0.01                                  | 0.0027±0.0002                                                                     |
|     | KE 220809-1c          | 20.00±0.01  | 100.0±0.4     | 278±3                             | 2.78±0.03                                  | 0.00345±0.00002                                                                   |
|     | KE 220809-1d          | 20.00±0.01  | 100.0±0.4     | 185±2                             | 1.85±0.02                                  | 0.003015±0.000004                                                                 |
|     | KE 220810-1a          | 20.00±0.01  | 100.0±0.4     | 339±4                             | 3.39±0.04                                  | 0.0033±0.0001                                                                     |
|     | KE 220810-1b          | 20.00±0.01  | 100.0±0.4     | 197±2                             | 1.97±0.02                                  | 0.00310±0.00009                                                                   |
| 110 | KE 220810-1c          | 20.00±0.01  | 100.0±0.4     | 247±3                             | 2.47±0.03                                  | 0.00341±0.00005                                                                   |
|     | KE 220810-1d          | 20.00±0.01  | 100.0±0.4     | 370±4                             | 3.70±0.04                                  | 0.00404±0.00003                                                                   |
|     | KE 220810-1e          | 20.00±0.01  | 100.0±0.4     | 123±1                             | 1.23±0.01                                  | 0.003100±0.000007                                                                 |



**Figure S1.** Plots of  $\ln(c_{g,0}/c_{g,t})$  versus  $t$  for PPN, observed in overnight experiments downstream from 50 mL of n-octanol at 5.00 °C for four different volumetric flow rates. Each data point shown is derived from the peak area of an individual chromatogram, of which there were between 119 and 219 at each flow rate. The data from Figure 3 are superimposed in black colour.



**Figure S2.** Plots of  $d\ln(c_{g,0}/c_{g,t})/dt$  versus  $\Phi/V_l$  for PPN in n-octanol at 20.00 °C (●), 12.50 °C (▲), and 5.00 °C (■).



**Figure S3.** Effect of adding Vitamin E on plots of  $d\ln(c_{g,0}/c_{g,t})/dt$  versus  $\Phi/V_l$  for PPN in n-octanol at 20.00 °C. Results with unadulterated n-octanol are shown as (■), whereas results with n-octanol containing  $\sim(0.6\pm0.2) \text{ mM}$  of  $\alpha\text{-tocopherol}$  are shown as (▲).

125 **Table S5.** Dimensionless Henry's law constants of PAN in deionized water,  $H_{S,aq}^{CC}(\text{PAN})$ . N/A = not  
available. n/d = not determined.

|                            | $H_{S,aq}^{CC}(\text{PAN})$<br>(unitless) |          |
|----------------------------|-------------------------------------------|----------|
| Reference                  | 293.15 K                                  | 278.15 K |
| (Lee, 1984)                | 98.3±4.8<br>(295 K)                       | n/d      |
| (Kames et al., 1991)       | 97.4±3.6                                  | N/A      |
| (Kames and Schurath, 1995) | 97.9±2.0                                  | N/A      |
| This work                  | 101±10                                    | 269±13   |

130 **Table S6.** Dimensionless Henry's law constants of PPN in deionized water,  $H_{S,aq}^{CC}(\text{PPN})$ . N/A = not  
available.

|                            | $H_{S,aq}^{CC}(\text{PPN})$<br>(unitless) |          |          |          |           |           |
|----------------------------|-------------------------------------------|----------|----------|----------|-----------|-----------|
| Reference                  | 298.15                                    | 293.15 K | 289.15 K | 285.65 K | 281.65 K  | 278.15 K  |
| (Kames and Schurath, 1995) | N/A                                       | 70.8±1.5 | N/A      | N/A      | N/A       | N/A       |
| This work                  | 36.5±1.1                                  | 64.2±4.4 | 74.5±4.5 | 96.4±1.7 | 114.7±7.1 | 160.1±5.6 |

**Table S7.** Dimensionless Henry's law constants of PPN in n-octanol,  $H_{S,oct}^{CC}(\text{PPN})$ .

|           | $H_{S,oct}^{CC}(\text{PPN})$<br>(unitless) |                                 |                                 |                                 |                                 |                                 |
|-----------|--------------------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| Reference | 298.15 K                                   | 293.15 K                        | 289.15 K                        | 285.65 K                        | 281.65 K                        | 278.15 K                        |
| This work | (2.15±0.11)<br>×10 <sup>3</sup>            | (2.35±0.21)<br>×10 <sup>3</sup> | (2.98±0.19)<br>×10 <sup>3</sup> | (3.07±0.18)<br>×10 <sup>3</sup> | (3.62±0.26)<br>×10 <sup>3</sup> | (4.65±0.36)<br>×10 <sup>3</sup> |

135 **Table S8.** Loss rate constants of PPN at 293.15 K.

| Compound and solvent / medium                                                      | $k$<br>( $10^{-4} \text{ s}^{-1}$ ) |
|------------------------------------------------------------------------------------|-------------------------------------|
| PPN in DI water                                                                    | 3.8±0.6                             |
| PPN in n-octanol                                                                   | 0.18±0.03                           |
| PPN in n-octanol containing $\sim(0.6\pm0.2) \text{ mM } \alpha\text{-tocopherol}$ | 0.40±0.04                           |
| PPN in air (Kabir et al., 2014)                                                    | 1.7                                 |

**Table S9a.** Estimated lifetimes of PAN with respect to wet deposition in the atmosphere at 293 K.

| Type                                      | $L$<br>( $\text{g m}^{-3}$ )              | $H_S^{\text{cc}}(\text{PAN}) \times L$ | $k_{\text{l, aq}}(\text{PAN})$<br>( $10^{-4} \text{ s}^{-1}$ ) | $\tau_{\text{wet}}(\text{PAN})$<br>$= (k_{\text{l, aq}} \times H_S^{\text{cc}} \times L)^{-1}$ |
|-------------------------------------------|-------------------------------------------|----------------------------------------|----------------------------------------------------------------|------------------------------------------------------------------------------------------------|
| Aerosol (low load)                        | $2.4 \times 10^{-6}$ (Nenes et al., 2021) | $2.4 \times 10^{-10}$                  | 3.8 (this work)                                                | 350 ky                                                                                         |
| Aerosol (high load)                       | $1.0 \times 10^{-4}$ (Nenes et al., 2021) | $1.0 \times 10^{-8}$                   | 3.8 (this work)                                                | 8.3 ky                                                                                         |
| Stratus clouds<br>(continental)           | 0.28 (Hess et al., 1998)                  | $2.8 \times 10^{-5}$                   | 3.8 (this work)                                                | 3.0 y                                                                                          |
| Stratus clouds<br>(maritime)              | 0.30 (Hess et al., 1998)                  | $3.0 \times 10^{-5}$                   | 44 (Kames and Schurath, 1995)                                  | 87 d                                                                                           |
| Cumulus clouds<br>(continental, clean)    | 0.26 (Hess et al., 1998)                  | $2.6 \times 10^{-5}$                   | 3.8 (this work)                                                | 3.2 y                                                                                          |
| Cumulus clouds<br>(continental, polluted) | 0.30 (Hess et al., 1998)                  | $3.0 \times 10^{-5}$                   | 3.8 (this work)                                                | 2.8 y                                                                                          |
| Cumulus clouds<br>(maritime)              | 0.44 (Hess et al., 1998)                  | $4.4 \times 10^{-5}$                   | 44 (Kames and Schurath, 1995)                                  | 59 d                                                                                           |
| Cumulonimbus<br>clouds (Java)             | 3.0 (Rosenfeld and Lensky, 1998)          | $3.0 \times 10^{-4}$                   | 3.8 (this work)                                                | 101 d                                                                                          |
| Fog                                       | 0.058 (Hess et al., 1998)                 | $5.8 \times 10^{-6}$                   | 3.8 (this work)                                                | 14 y                                                                                           |
| Fog (Po Valley)                           | 0.3 (Wobrock et al., 1992)                | $3.0 \times 10^{-5}$                   | 3.8 (this work)                                                | 2.8 y                                                                                          |
| Fog (maritime)                            | 0.058 (Hess et al., 1998)                 | $5.8 \times 10^{-6}$                   | 44 (Kames and Schurath, 1995)                                  | 1.2 y                                                                                          |
| Fog (maritime)                            | 0.8 (Dimitrova et al., 2021)              | $8.1 \times 10^{-5}$                   | 44 (Kames and Schurath, 1995)                                  | 33 d                                                                                           |
| Fog (maritime)                            | 1.8 (Osthoff et al., 2006)                | $1.8 \times 10^{-4}$                   | 44 (Kames and Schurath, 1995)                                  | 14 d                                                                                           |

**Table S9b.** Estimated lifetimes of PPN with respect to wet deposition in the atmosphere at 293 K.

| Type                                      | $L$<br>(g m <sup>-3</sup> )               | $H_S^{cc}(\text{PPN}) \times L$ | $k_{l,aq}(\text{PPN})$<br>(10 <sup>-4</sup> s <sup>-1</sup> ) | $\tau_{\text{wet}}(\text{PPN})$<br>$= (k_{l,aq} \times H_S^{cc} \times L)^{-1}$ |
|-------------------------------------------|-------------------------------------------|---------------------------------|---------------------------------------------------------------|---------------------------------------------------------------------------------|
| Aerosol (low load)                        | 2.4×10 <sup>-6</sup> (Nenes et al., 2021) | 1.5 ×10 <sup>-10</sup>          | 3.8 (this work)                                               | 540 ky                                                                          |
| Aerosol (high load)                       | 1.0×10 <sup>-4</sup> (Nenes et al., 2021) | 6.4 ×10 <sup>-9</sup>           | 3.8 (this work)                                               | 13 ky                                                                           |
| Stratus clouds<br>(continental)           | 0.28 (Hess et al., 1998)                  | 1.8 ×10 <sup>-5</sup>           | 3.8 (this work)                                               | 4.6 y                                                                           |
| Stratus clouds<br>(maritime)              | 0.30 (Hess et al., 1998)                  | 1.9 ×10 <sup>-5</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 137 d                                                                           |
| Cumulus clouds<br>(continental, clean)    | 0.26 (Hess et al., 1998)                  | 1.7 ×10 <sup>-5</sup>           | 3.8 (this work)                                               | 5.0 y                                                                           |
| Cumulus clouds<br>(continental, polluted) | 0.30 (Hess et al., 1998)                  | 1.9 ×10 <sup>-5</sup>           | 3.8 (this work)                                               | 4.3 y                                                                           |
| Cumulus clouds<br>(maritime)              | 0.44 (Hess et al., 1998)                  | 2.8 ×10 <sup>-5</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 93 d                                                                            |
| Cumulonimbus<br>clouds (Java)             | 3.0 (Rosenfeld and Lensky,<br>1998)       | 1.9 ×10 <sup>-4</sup>           | 3.8 (this work)                                               | 158 d                                                                           |
| Fog                                       | 0.058 (Hess et al., 1998)                 | 3.7 ×10 <sup>-6</sup>           | 3.8 (this work)                                               | 22 y                                                                            |
| Fog (Po Valley)                           | 0.3 (Wobrock et al., 1992)                | 1.9 ×10 <sup>-5</sup>           | 3.8 (this work)                                               | 4.3 y                                                                           |
| Fog (maritime)                            | 0.058 (Hess et al., 1998)                 | 3.7 ×10 <sup>-6</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 1.9 y                                                                           |
| Fog (maritime)                            | 0.8 (Dimitrova et al., 2021)              | 5.1 ×10 <sup>-5</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 51 d                                                                            |
| Fog (maritime)                            | 1.8 (Osthoff et al., 2006)                | 1.2 ×10 <sup>-4</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 23 d                                                                            |

**Table S10a.** Estimated lifetimes of PAN with respect to wet deposition in the atmosphere at 278 K.

| Type                                      | $L$<br>(g m <sup>-3</sup> )               | $H_S^{cc}(\text{PAN}) \times L$ | $k_{l,aq}(\text{PAN})$<br>(10 <sup>-4</sup> s <sup>-1</sup> ) | $\tau_{wet}(\text{PAN})$<br>$= (k_{l,aq} \times H_S^{cc} \times L)^{-1}$ |
|-------------------------------------------|-------------------------------------------|---------------------------------|---------------------------------------------------------------|--------------------------------------------------------------------------|
| Aerosol (low load)                        | 2.4×10 <sup>-6</sup> (Nenes et al., 2021) | 6.4 ×10 <sup>-10</sup>          | 1.8 (this work)                                               | 274 ky                                                                   |
| Aerosol (high load)                       | 1.0×10 <sup>-4</sup> (Nenes et al., 2021) | 2.7 ×10 <sup>-8</sup>           | 1.8 (this work)                                               | 6.5 ky                                                                   |
| Stratus clouds<br>(continental)           | 0.28 (Hess et al., 1998)                  | 7.5 ×10 <sup>-5</sup>           | 1.8 (this work)                                               | 2.3 y                                                                    |
| Stratus clouds<br>(maritime)              | 0.30 (Hess et al., 1998)                  | 8.1 ×10 <sup>-5</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 33 d                                                                     |
| Cumulus clouds<br>(continental, clean)    | 0.26 (Hess et al., 1998)                  | 7.0 ×10 <sup>-5</sup>           | 1.8 (this work)                                               | 2.5 y                                                                    |
| Cumulus clouds<br>(continental, polluted) | 0.30 (Hess et al., 1998)                  | 8.1 ×10 <sup>-5</sup>           | 1.8 (this work)                                               | 2.2 y                                                                    |
| Cumulus clouds<br>(maritime)              | 0.44 (Hess et al., 1998)                  | 1.2 ×10 <sup>-4</sup>           | 44 (Kames and<br>Schurath, 1995)                              | 22 d                                                                     |
| Cumulonimbus<br>clouds (Java)             | 3.0 (Rosenfeld and Lensky,<br>1998)       | 8.1 ×10 <sup>-4</sup>           | 1.8 (this work)                                               | 80 d                                                                     |
| Fog                                       | 0.058 (Hess et al., 1998)                 | 1.6 ×10 <sup>-5</sup>           | 1.8 (this work)                                               | 11 y                                                                     |
| Fog (Po Valley)                           | 0.3 (Wobrock et al., 1992)                | 8.1 ×10 <sup>-5</sup>           | 1.8 (this work)                                               | 2.2 y                                                                    |
| Fog (maritime)                            | 0.058 (Hess et al., 1998)                 | 1.6×10 <sup>-5</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 168 d                                                                    |
| Fog (maritime)                            | 0.8 (Dimitrova et al., 2021)              | 2.2×10 <sup>-4</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 12 d                                                                     |
| Fog (maritime)                            | 1.8 (Osthoff et al., 2006)                | 4.8×10 <sup>-4</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 5 d                                                                      |

**Table S10b.** Estimated lifetimes of PPN with respect to wet deposition in the atmosphere at 278 K.

| Type                                      | $L$<br>(g m <sup>-3</sup> )               | $H_S^{cc}(\text{PPN}) \times L$ | $k_{l,aq}(\text{PPN})$<br>(10 <sup>-4</sup> s <sup>-1</sup> ) | $\tau_{wet}(\text{PPN})$<br>$= (k_{l,aq} \times H_S^{cc} \times L)^{-1}$ |
|-------------------------------------------|-------------------------------------------|---------------------------------|---------------------------------------------------------------|--------------------------------------------------------------------------|
| Aerosol (low load)                        | 2.4×10 <sup>-6</sup> (Nenes et al., 2021) | 3.8×10 <sup>-10</sup>           | 1.0 (this work)                                               | 840 ky                                                                   |
| Aerosol (high load)                       | 1.0×10 <sup>-4</sup> (Nenes et al., 2021) | 1.6×10 <sup>-8</sup>            | 1.0 (this work)                                               | 20 ky                                                                    |
| Stratus clouds<br>(continental)           | 0.28 (Hess et al., 1998)                  | 4.5×10 <sup>-5</sup>            | 1.0 (this work)                                               | 7.2 y                                                                    |
| Stratus clouds<br>(maritime)              | 0.30 (Hess et al., 1998)                  | 4.8×10 <sup>-5</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 55 d                                                                     |
| Cumulus clouds<br>(continental, clean)    | 0.26 (Hess et al., 1998)                  | 4.2×10 <sup>-5</sup>            | 1.0 (this work)                                               | 7.7 y                                                                    |
| Cumulus clouds<br>(continental, polluted) | 0.30 (Hess et al., 1998)                  | 4.8×10 <sup>-5</sup>            | 1.0 (this work)                                               | 6.7 y                                                                    |
| Cumulus clouds<br>(maritime)              | 0.44 (Hess et al., 1998)                  | 7.0×10 <sup>-5</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 37 d                                                                     |
| Cumulonimbus<br>clouds (Java)             | 3.0 (Rosenfeld and Lensky,<br>1998)       | 4.8×10 <sup>-4</sup>            | 1.0 (this work)                                               | 244 d                                                                    |
| Fog                                       | 0.058 (Hess et al., 1998)                 | 9.3×10 <sup>-6</sup>            | 1.0 (this work)                                               | 35 y                                                                     |
| Fog (Po Valley)                           | 0.3 (Wobrock et al., 1992)                | 4.8×10 <sup>-5</sup>            | 1.0 (this work)                                               | 6.7 y                                                                    |
| Fog (maritime)                            | 0.058 (Hess et al., 1998)                 | 9.3×10 <sup>-6</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 283 d                                                                    |
| Fog (maritime)                            | 0.8 (Dimitrova et al., 2021)              | 1.3×10 <sup>-4</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 21 d                                                                     |
| Fog (maritime)                            | 1.8 (Osthoff et al., 2006)                | 2.9×10 <sup>-4</sup>            | 44 (Kames and<br>Schurath, 1995)                              | 9 d                                                                      |

145 **Table S11.** Reactive uptake probabilities of PAN and PPN calculated using Eq. (9-10). The water viscosities were obtained from Korson et al. (1969) and those for n-octanol were calculated by linear extrapolation of the above-room temperature data by Venkatesan et al. (2020). Molar volume data were obtained using the PhysChem module of the ACD/Labs percepta platform via the Royal Society of Chemistry's Chemspider web site (2022).

| Compound and solvent | $T$<br>(K) | $\mu$<br>(mPa s) | $D_l$<br>( $10^{-9} \text{ m}^2 \text{ s}^{-1}$ ) | $k_l$<br>( $10^{-5} \text{ s}^{-1}$ ) | $\omega$<br>( $\text{m s}^{-1}$ ) | $H_S^{CC}$ | $\gamma$<br>( $10^{-5}$ ) |
|----------------------|------------|------------------|---------------------------------------------------|---------------------------------------|-----------------------------------|------------|---------------------------|
| PAN and DI water     | 278.15     | 1.5192           | 0.88                                              | 18                                    | 221                               | 269        | 0.2                       |
| PAN and DI water     | 293.15     | 1.0020           | 1.4                                               | 38                                    | 226                               | 101        | 0.1                       |
| PPN and DI water     | 278.15     | 1.5192           | 0.86                                              | 10                                    | 209                               | 160        | 0.09                      |
| PPN and DI water     | 293.15     | 1.0020           | 1.4                                               | 38                                    | 214                               | 64         | 0.09                      |
| PAN and n-octanol    | 278.15     | 12.2             | 2.3                                               | 0.5                                   | 221                               | 1920       | 0.4                       |
| PAN and n-octanol    | 293.15     | 9.3              | 3.2                                               | 0.3                                   | 226                               | 1010       | 0.2                       |
| PPN and n-octanol    | 278.15     | 12.2             | 2.3                                               | 0.3                                   | 209                               | 4652       | 0.7                       |
| PPN and n-octanol    | 293.15     | 9.3              | 3.2                                               | 1.8                                   | 214                               | 2351       | 1.1                       |

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