

5 **Table S1: Estimated sub-cooled liquid saturation vapour pressures at 298 K. N_Vp (Nannoolal vapour pressure), MY_Vp (Myrdal and Yalkowsky vapour pressure), EVAPORATION (EVAPORATION vapour pressure), SIMPOL (SIMPOL vapour pressure), N_Tb (Nannoolal boiling point), SB_Tb (Stein and Brown boiling point), Literature (2-nitrophenol, 3-methyl-2-nitrophenol, 4-methyl-2-nitrophenol, 5-fluoro-2-nitrophenol, 4-nitrophenol from (Schwarzenbach et al., 1988), 3-nitrophenol from (Ribeiro da Silva et al., 1992) 2-nitrobenzaldehyde, 3-nitrobenzaldehyde from (Perry et al., 1984), 2-nitrobenzoic acid, 3-nitrobenzoic acid, 4-nitrobenzoic acid from (Ribeiro Da Silva et al., 1999), 4-methyl-3-nitrobenzoic acid, 3-methyl-4-nitrobenzoic acid from (Monte et al., 2001)) - literature data for previous KEMS work (3-nitrophenol, 4-nitrophenol from (Bannan et al., 2017), 4-methyl-2-nitrophenol, 4-methyl-3-nitrophenol, 3-methyl-4-nitrophenol from (Dang et al., 2019)). This table contains the corresponding information used in Fig. 8.**

Compound	N_Vp & N_Tb (Pa)	N_Vp & SB_Tb (Pa)	MY_Vp & N_Tb (Pa)	MY_Vp & SB_Tb (Pa)	SIMPOL (Pa)	EVAPORATION (Pa)	Literature (Pa)	Literature (previous KEMS studies) (Pa)	Experimental (Pa)
2-nitrophenol	1.37E+03	1.80E+02	1.13E+03	1.22E+02	3.58E+01	1.37E+04	2.69E+01	nan	1.38E-03
3-methyl-2-nitrophenol	3.58E+02	5.53E+01	3.25E+02	4.49E+01	1.35E+01	4.47E+03	1.12E+01	nan	1.22E-02
4-methyl-2-nitrophenol	3.58E+02	5.53E+01	3.25E+02	4.49E+01	1.35E+01	4.47E+03	9.63E+00	5.97E-04	3.29E-03
5-fluoro-2-nitrophenol	1.03E+03	1.98E+02	9.67E+02	1.68E+02	3.58E+01	1.37E+04	3.05E+00	nan	5.01E-03
4-amino-2-nitrophenol	6.70E+00	2.36E+00	6.79E+00	2.36E+00	9.35E-01	1.37E+04	nan	nan	9.29E-02
3-nitrophenol	1.11E+03	1.70E+02	9.37E+02	1.22E+02	3.58E+01	1.37E+04	9.40E-02	1.14E-02	nan
4-methyl-3-nitrophenol	3.58E+02	5.53E+01	3.25E+02	4.49E+01	1.35E+01	4.47E+03	nan	4.85E-03	6.85E-02
4-chloro-3-nitrophenol	2.09E+02	3.22E+01	1.87E+02	2.58E+01	3.58E+01	1.37E+04	nan	nan	5.80E-02
4-nitrophenol	9.60E+02	1.69E+02	8.04E+02	1.22E+02	3.58E+01	1.37E+04	1.95E-01	5.14E-03	nan
3-methyl-4-nitrophenol	3.58E+02	5.53E+01	3.25E+02	4.49E+01	1.35E+01	4.47E+03	nan	3.78E-03	5.86E-02
2-fluoro-4-	1.03E+03	1.98E+02	9.67E+02	1.68E+02	3.58E+01	1.37E+04	nan	nan	6.42E-02

nitrophenol									
3-fluoro-4-nitrophenol	1.03E+03	1.98E+02	9.67E+02	1.68E+02	3.58E+01	1.37E+04	nan	nan	3.32E-02
2-nitrobenzaldehyde	8.33E+02	1.56E+02	7.94E+02	1.33E+02	6.08E-01	2.86E+02	2.39E+00	nan	2.15E+00
3-nitrobenzaldehyde	6.80E+02	1.46E+02	6.73E+02	1.33E+02	6.08E-01	2.86E+02	9.70E-01	nan	2.75E-01
2-chloro-5-nitrobenzaldehyde	1.46E+02	3.04E+01	1.45E+02	2.83E+01	6.08E-01	2.86E+02	nan	nan	8.41E-02
4-nitrobenzaldehyde	5.95E+02	1.45E+02	5.87E+02	1.33E+02	6.08E-01	2.86E+02	nan	nan	1.93E-01
2-nitrobenzoic acid	1.12E+01	9.32E-01	2.28E+01	2.18E+00	3.91E-03	1.09E+00	4.44E-03	nan	nan
5-chloro-2-nitrobenzoic acid	1.42E+00	1.50E-01	4.48E+00	5.85E-01	3.91E-03	1.09E+00	nan	nan	1.40E-02
3-nitrobenzoic acid	8.59E+00	8.48E-01	1.90E+01	2.18E+00	3.91E-03	1.09E+00	5.05E-03	nan	1.90E-03
4-methyl-3-nitrobenzoic acid	2.56E+00	2.52E-01	7.63E+00	9.26E-01	1.47E-03	3.57E-01	3.07E-03	nan	5.76E-02
2-chloro-3-nitrobenzoic acid	1.42E+00	1.50E-01	4.48E+00	5.85E-01	3.91E-03	1.09E+00	nan	nan	6.29E-03
2-hydroxy-5-nitrobenzoic acid	1.15E+00	1.35E-02	5.50E+00	1.18E-01	4.16E-03	1.09E+00	nan	nan	1.87E-02
4-nitrobenzoic acid	7.28E+00	8.42E-01	1.64E+01	2.18E+00	3.91E-03	1.09E+00	1.94E-02	nan	nan
3-methyl-4-nitrobenzoic acid	2.56E+00	2.52E-01	7.63E+00	9.26E-01	1.47E-03	3.57E-01	7.71E-03	nan	3.04E-01

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