Table 1S: Essential Molecular Parameters of Species for Estimation of Gas Diffusion Coefficients

	T_b (K) [a]	V_b (cm^3/mol) [c]	$\Sigma\nu$ [d]	μ (D) [e]	σ (Å) [h]	ε/k_b (K) [k]
Helium					2.55 [i]	10 [l]
Water	373.2 [b]	18.7	13.1	1.85 [f]	2.64 [i]	809 [l]
2-Nitrophenol	490.4 [b]	130.1	111.5	6.35 [g]	5.98 [j]	564 [m]
2-Methylphenol	464.3 [b]	125.6	117.6	1.45 [f]	5.91 [j]	534 [m]
3-Methylphenol	475.2 [b]	125.6	117.6	1.48 [f]	5.91 [j]	546 [m]
4-Methylphenol	475.0 [b]	125.6	117.6	1.48 [f]	5.91 [j]	546 [m]

[a] T_b is the normal boiling point (at 1 atm). [b] NIST Webbook (ref 1S). [C] V_b is the liquid molar volume found from experimental data or estimated from the Le Bas contributions (presented in Table 3-8 in ref 2S). [d] $\Sigma\nu$ is the sum of atomic and structural diffusion volume increments (presented in Table 11-1 in ref 2S). [e] μ is the dipole moment. [f] values taken from ref 3S. [g] value estimated by Guanghua et al. (ref 4S). [h] σ is the characteristic Lennard-Jones length. [i] values from Appendix B (ref 2S). [j] values estimated by eq. 11-4.2 (ref 2S). [k] ε/k_b is the characteristic Lennard-Jones energy. [l] values from Appendix B (ref 2S). [m] values estimated by eq. 11-4.3 (ref 2S).

Table 2S: Pressure-Independent Diffusion Coefficients of Phenolic Compounds in Water and Helium using the method of Brokaw (ref 5S)

T **(K)**	**2-Nitrophenol**		**2-Methylphenol**		**3-Methylphenol**		**4-Methylphenol**	
	D_g(X/H_2O) (Torr cm^2/s)	D_g (X/He) (Torr cm^2/s)	D_g(X/H_2O) (Torr cm^2/s)	D_g (X/He) (Torr cm^2/s)	D_g(X/H_2O) (Torr cm^2/s)	D_g (X/He) (Torr cm^2/s)	D_g(X/H_2O) (Torr cm^2/s)	D_g (X/He) (Torr cm^2/s)
278			49.8	207.2				
283	42.7	208.1	51.6	213.7	51.3	213.2	51.3	213.2
288	44.2	214.5	53.5	220.3	53.2	219.7	53.2	219.7
293	45.8	221.0	55.3	227.0	55.0	226.4	55.0	226.4
298	47.4	227.6	57.3	233.7	56.9	233.1	56.9	233.1
303							58.8	239.9

Table 3S: Mass Accommodation Coefficients of the Studied Phenolic Compounds Over the Temperature Range of Interest using binary gas diffusion coefficients estimated by the method of Brokaw[a]

T **(K)**	**2-Nitrophenol**	**2-Methylphenol**	**3-Methylphenol**	**4-Methylphenol**
278		$(2.9 \pm 0.2) \times 10^{-3}$		
283	$(5.5 \pm 0.9) \times 10^{-3}$	$(2.3 \pm 0.3) \times 10^{-3}$	$(3.2 \pm 0.5) \times 10^{-3}$	$(4.6 \pm 0.4) \times 10^{-3}$
288	$(4.0 \pm 1.2) \times 10^{-3}$	$(1.1 \pm 0.1) \times 10^{-3}$	$(2.6 \pm 0.3) \times 10^{-3}$	$(3.6 \pm 0.3) \times 10^{-3}$
293	$(1.5 \pm 0.4) \times 10^{-3}$	$(6.7 \pm 0.3) \times 10^{-4}$	$(1.5 \pm 0.5) \times 10^{-3}$	$(2.3 \pm 0.2) \times 10^{-3}$
298	$(1.0 \pm 0.1) \times 10^{-3}$	$(3.2 \pm 0.4) \times 10^{-4}$	$(7.3 \pm 0.9) \times 10^{-4}$	$(1.2 \pm 0.2) \times 10^{-3}$
303				$(6.1 \pm 0.6) \times 10^{-4}$

[a] The given errors are calculated with a 95% confidence interval limit using the student's *t*-distribution.

References for Supporting Information

(1S) NIST Chemistry Webbook, NIST Standard Reference Database Number 69 – March 2003 Release

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(4S) Guanghua, L.; Jie, T.; Xing, Y.; Yuanhui, Z. *Chemical Journal on Internet*, **2001**, *3*, 34.

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