Supplemental information for

Measurement of octanol-air and air-water partition coefficients of isopropyl and isobutyl nitrate

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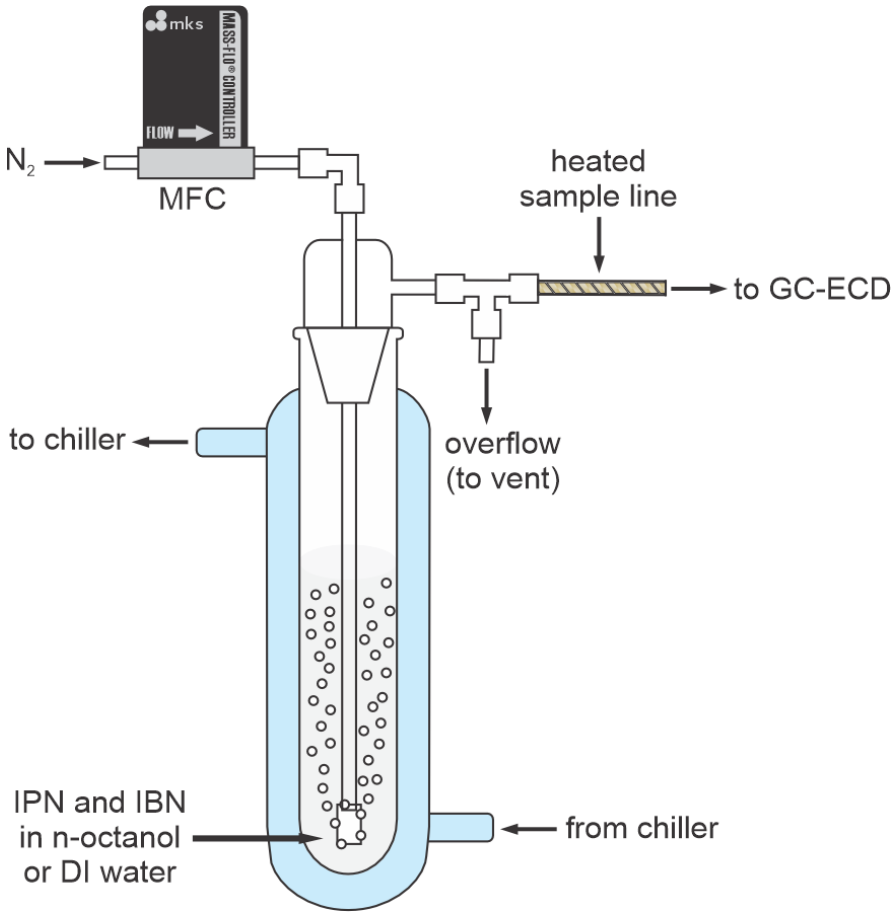

Figure S1. Schematic of the jacketed bubble column apparatus (not to scale). MFC = mass flow controller. GC-ECD = gas chromatograph with electron capture detection. DI water = deionized water.

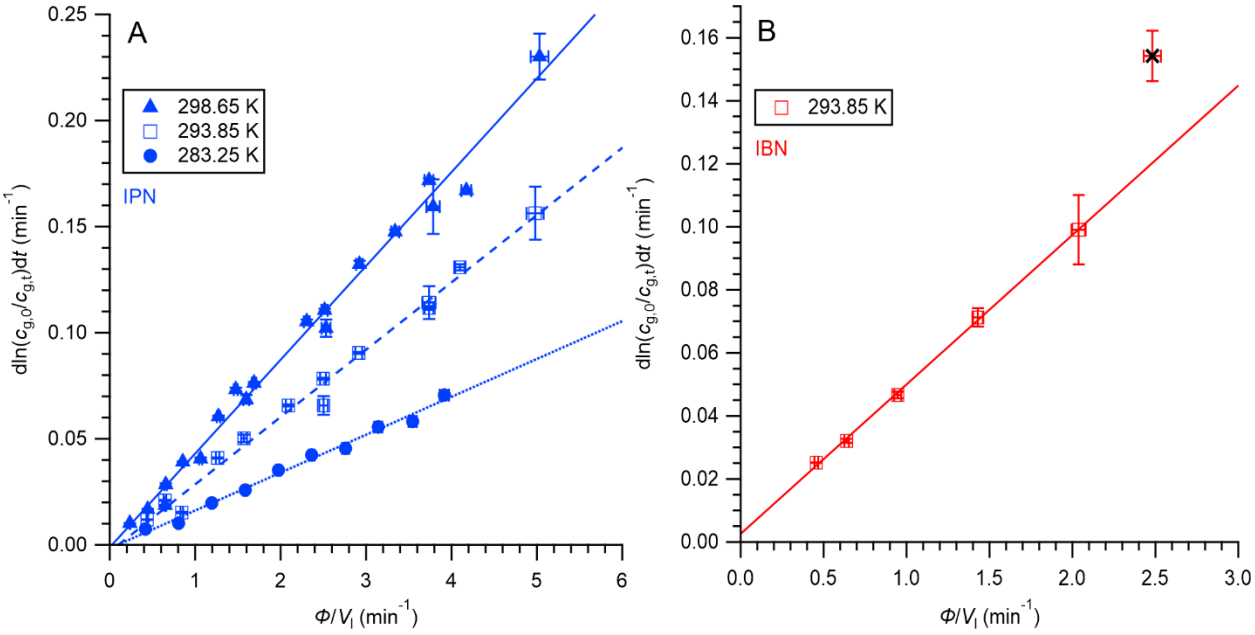

Figure S2. Plots of dln($c_{g,0}/c_{g,t}$)/dt versus Φ/V_l for (A) IPN and (B) IBN in DI water. The IBN datum suspected to have not achieved equilibrium (crossed out in Table S3) is shown as a bolded cross (×) symbol. The straight lines are linear fits to the data at each temperature. Error bars are ±1σ precision.

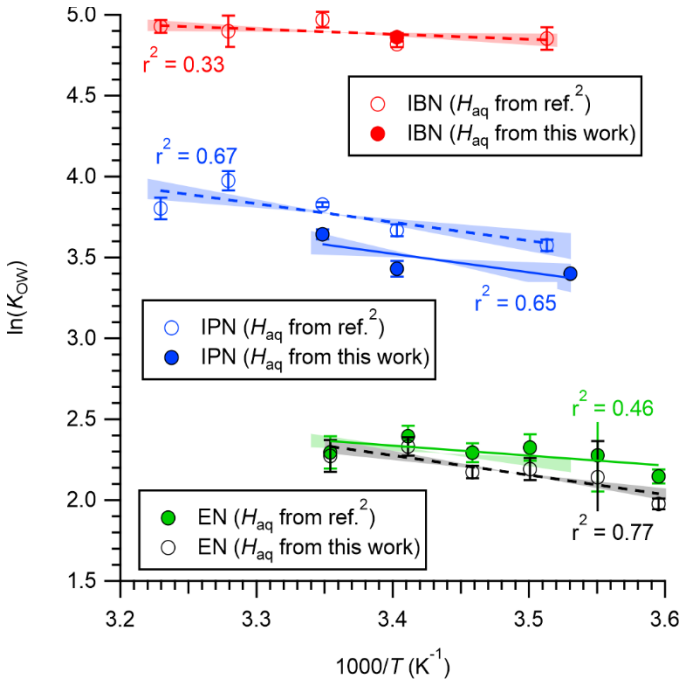

Figure S3. Natural logarithm of the octanol-water partition coefficients (K_{OW}) of IPN, IBN, and EN as a function of 1000/*T*. All K_{OW} values shown were calculated according to Eq. (2). For IPN (blue colour) and IBN (red colour), the solid symbols (●) represent K_{OW} values calculated using H_{oct} and H_{aq} values measured in this work. For EN, the solid symbols (●, green colour) represent K_{OW} values calculated using H_{oct} and H_{aq} measured by Easterbrook et al.[1] The open symbols (○) represent K_{OW} values calculated using H_{aq} values derived from the temperature dependence parameterizations of IPN, IBN, and EN reported by Kames and Schurath.[2] The lines are linear fits to the data. The shaded regions represent upper and lower error bounds for each linear fit, i.e., $\ln(K_{OW}) = (m+\sigma_m)/T + (b-\sigma_b)$ and $\ln(K_{OW}) = (m-\sigma_m)/T + (b+\sigma_b)$. Error bars are ±1σ precision.

Table S1. Overview of experimental conditions for IPN and IBN in n-octanol. Uncertainties are at the ±1σ level. The $d\ln(c_{g,0}/c_{g,t})/dt$ data marked with a dash (-) indicates that the specified compound was not present.

Internal reference	$T_{setpoint}$ (°C)	$T_{corrected}$ (°C)	V_l (mL)	Φ (mL min^{-1})	$\frac{\Phi}{V_l}$ (min^{-1})	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ for IPN (10^3 min^{-1})	r (%)	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ for IBN (10^3 min^{-1})	r (%)
KE 240705-3	25.00±0.01	25.5±0.5	100.0±0.6	190±1	1.90±0.02	2.391±0.008	99.73	1.094±0.003	99.69
KL 240708-3	25.00±0.01	25.5±0.5	100.0±0.6	159±1	1.59±0.01	-	-	0.752±0.007	99.55
KL 240710-2	25.00±0.01	25.5±0.5	100.0±0.6	505±2	5.05±0.03	0.005.81±0.01	99.99	-	-
KL 240711-1	25.00±0.01	25.5±0.5	100.0±0.6	316±1	3.16±0.02	3.87±0.02	99.93	-	-
KL 240711-2	25.00±0.01	25.5±0.5	100.0±0.6	565±2	5.65±0.04	6.44±0.02	99.96	2.412±0.006	99.97
KL 240712-2	25.00±0.01	25.5±0.5	100.0±0.6	253±1	2.53±0.02	3.109±0.006	99.97	1.140±0.002	99.95
KL 240717	25.00±0.01	25.5±0.5	100.0±0.6	65±1	0.65±0.01	0.713±0.003	99.83	-	-
KL 240718	25.00±0.01	25.5±0.5	100.0±0.6	439±2	4.39±0.03	5.23±0.01	99.98	1.890±0.003	99.99
KL 240719	25.00±0.01	25.5±0.5	150.0±2.0	65±1	0.43±0.01	0.513±0.001	99.96	-	-
KL 240722	25.00±0.01	25.5±0.5	150.0±2.0	347±1	2.31±0.03	2.70±0.01	99.94	0.955±0.003	99.95
KL 240724	25.00±0.01	25.5±0.5	150.0±2.0	147±1	0.98±0.01	1.115±0.001	99.99	0.383±0.003	99.75
KL 240725-1	25.00±0.01	25.5±0.5	150.0±2.0	537±2	3.58±0.05	4.25±0.01	99.98	1.531±0.007	99.95
KL 240725-2	25.00±0.01	25.5±0.5	150.0±2.0	443±2	2.96±0.04	3.489±0.006	99.99	1.328±0.003	99.99
KL 240726	25.00±0.01	25.5±0.5	150.0±2.0	224±1	1.49±0.02	1.793±0.004	99.91	0.6484±0.0009	99.97
KL 240729	25.00±0.01	25.5±0.5	150.0±2.0	570±2	3.80±0.05	4.554±0.008	99.99	1.632±0.002	99.99
AB 241009-1	20.00±0.01	20.7±0.5	100.0±2.0	403±2	4.03±0.08	3.78±0.01	99.97	1.424±0.008	99.83
AB 241010-1	20.00±0.01	20.7±0.5	100.0±2.0	95±1	0.95±0.02	0.86±0.03	98.28	0.31±0.03	91.10
AB 241010-2	20.00±0.01	20.7±0.5	100.0±2.0	187±1	1.87±0.04	1.765±0.006	99.93	0.620±0.002	99.95
AB 241011-1	20.00±0.01	20.7±0.5	100.0±2.0	64±1	0.64±0.01	0.613±0.002	99.95	0.221±0.001	99.68
AB 241015-1	20.00±0.01	20.7±0.5	100.0±2.0	498±2	4.98±0.10	4.68±0.02	99.97	1.79±0.01	99.86
AB 241126-2	37.00±0.01	36.5±0.5	100.0±2.0	68±1	0.68±0.02	1.530±0.010	99.87	0.91±0.03	96.12
AB 241127-1	37.00±0.01	36.5±0.5	100.0±2.0	426±2	4.26±0.09	9.5±0.2	99.76	3.38±0.07	99.51
AB 241127-2	37.00±0.01	36.5±0.5	100.0±2.0	133±1	1.33±0.03	2.82±0.01	99.97	1.26±0.03	98.19
AB 241128-1	37.00±0.01	36.5±0.5	100.0±2.0	589±2	5.89±0.12	13.4±0.2	99.76	4.9±0.1	99.11
AB 241129-1	37.00±0.01	36.5±0.5	100.0±2.0	296±1	2.96±0.06	7.3±0.1	99.29	2.57±0.02	99.84
KE 250106-2	32.00±0.01	31.8±0.5	100.0±2.0	130±1	1.30±0.03	1.91±0.05	97.17	0.555±0.009	98.66
KE 250107-1	32.00±0.01	31.8±0.5	100.0±2.0	576±2	5.76±0.12	8.31±0.06	99.93	3.53±0.08	98.83
KE 250107-2	32.00±0.01	31.8±0.5	100.0±2.0	387±2	3.87±0.08	5.73±0.05	99.85	3.1±0.1	93.88

Table S1 (continued). Overview of experimental conditions for IPN and IBN in n-octanol. Uncertainties are at the ±1σ level. The $d\ln(c_{g,0}/c_{g,t})/dt$ data marked with a dash (-) indicates that the specified compound was not present.

Internal reference	$T_{setpoint}$ (°C)	$T_{corrected}$ (°C)	V_l (mL)	Φ (mL min^{-1})	$\frac{\Phi}{V_l}$ (min^{-1})	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ for IPN (10^3 min^{-1})	r (%)	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ for IBN (10^3 min^{-1})	r (%)
KE 250108-1	32.00±0.01	31.8±0.5	100.0±2.0	481±2	4.81±0.10	7.08±0.06	99.83	2.77±0.04	98.92
KE 250109-1	32.00±0.01	31.8±0.5	100.0±2.0	323±1	3.23±0.07	4.68±0.03	99.91	1.82±0.02	98.97
KE 250110-1	32.00±0.01	31.8±0.5	100.0±2.0	229±1	2.29±0.05	3.55±0.02	99.88	1.323±0.005	99.87
KE 250113-1	32.00±0.01	31.8±0.5	100.0±2.0	419±2	4.19±0.09	6.42±0.05	99.88	2.33±0.03	99.50
KE 250121-1	10.00±0.01	11.5±0.5	100.0±2.0	299±1	2.99±0.06	2.04±0.02	99.63	0.75±0.02	94.97
KE 250122-1	10.00±0.01	11.5±0.5	100.0±2.0	475±2	4.75±0.10	3.17±0.03	99.87	1.04±0.01	99.24
KE 250123-1	10.00±0.01	11.5±0.5	100.0±2.0	359±1	3.59±0.07	2.48±0.05	99.45	0.81±0.02	97.38
KE 250124-1	10.00±0.01	11.5±0.5	100.0±2.0	180±1	1.80±0.04	1.214±0.008	99.63	0.415±0.007	97.77
KE 250125-1	10.00±0.01	11.5±0.5	100.0±2.0	417±2	4.17±0.08	2.74±0.02	99.82	0.93±0.01	98.27
KE 250127-1	10.00±0.01	11.5±0.5	100.0±2.0	240±1	2.40±0.05	1.70±0.01	99.71	0.58±0.01	97.73
KE 250129-1	20.00±0.01	20.7±0.5	100.0±2.0	252±1	2.52±0.05	-	-	0.80±0.02	96.75
KE 250130-1	20.00±0.01	20.7±0.5	100.0±2.0	562±2	5.62±0.11	5.98±0.04	99.95	2.06±0.05	99.24
KE 250131-1	20.00±0.01	20.7±0.5	100.0±2.0	157±1	1.57±0.03	1.64±0.01	99.81	0.550±0.003	99.50
KE 250203-1	20.00±0.01	20.7±0.5	100.0±2.0	339±1	3.39±0.07	3.50±0.04	99.15	1.23±0.01	99.45
KE 250204-1	20.00±0.01	20.7±0.5	100.0±2.0	280±1	2.80±0.06	2.84±0.02	99.87	1.007±0.006	99.75
KE 250205-1	20.00±0.01	20.7±0.5	100.0±2.0	96±1	0.96±0.02	1.010±0.006	99.85	0.37±0.01	95.61
KE 250206-1	20.00±0.01	20.7±0.5	100.0±2.0	465±2	4.65±0.09	5.01±0.04	99.90	1.67±0.01	99.66
KE 250207-1	37.00±0.01	36.5±0.5	100.0±2.0	229±1	2.29±0.05	4.97±0.05	99.86	1.77±0.01	99.73
KE 250210-1	37.00±0.01	36.5±0.5	100.0±2.0	488±2	4.88±0.10	9.51±0.09	99.88	4.06±0.05	99.76
KE 250211-1	37.00±0.01	36.5±0.5	100.0±2.0	362±1	3.62±0.07	7.28±0.06	99.91	3.14±0.03	99.78
KE 250212-1	32.00±0.01	31.8±0.5	100.0±2.0	164±1	1.64±0.03	3.22±0.04	99.71	1.11±0.02	98.28
KE 250213-1	32.00±0.01	31.8±0.5	100.0±2.0	67±1	0.67±0.02	1.131±0.005	99.80	0.443±0.003	98.73
KE 250218-1	32.00±0.01	31.8±0.5	100.0±2.0	360±1	3.60±0.07	6.39±0.09	99.79	2.41±0.05	97.06

Table S2. Overview of experimental conditions for IPN in DI water. Uncertainties are at the ±1σ level.

Internal reference	$T_{setpoint}$ (°C)	$T_{corrected}$ (°C)	V_l (mL)	Φ (mL min^{-1})	$\frac{\Phi}{V_l}$ (min^{-1})	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min^{-1})	r (%)
KL 240731	25.00±0.01	25.5±0.5	150.0±2.0	67±1	0.44±0.01	0.0167±0.0002	99.89
KL 240801-1	25.00±0.01	25.5±0.5	150.0±2.0	626±3	4.17±0.06	0.1670±0.0006	100.0
KL 240801-2	25.00±0.01	25.5±0.5	150.0±2.0	253±2	1.69±0.02	0.0763±0.0004	99.98
KL 240801-3	25.00±0.01	25.5±0.5	150.0±2.0	377±2	2.51±0.04	0.1106±0.0008	99.98
KL 240801-4	25.00±0.01	25.5±0.5	150.0±2.0	97±1	0.65±0.01	0.0186±0.0003	99.81
KL 240802-1	25.00±0.01	25.5±0.5	150.0±2.0	128±1	0.85±0.01	0.0392±0.0002	99.99
KL 240802-2	25.00±0.01	25.5±0.5	150.0±2.0	35±1	0.23±0.01	0.01029±0.00003	99.91
KL 240806-1	25.00±0.01	25.5±0.5	150.0±2.0	346±2	2.31±0.03	0.1052±0.0010	99.97
KL 240806-2	25.00±0.01	25.5±0.5	150.0±2.0	191±1	1.27±0.02	0.0605±0.0005	99.99
KL 240806-3	25.00±0.01	25.5±0.5	150.0±2.0	501±2	3.34±0.05	0.1477±0.0010	99.99
KL 240806-4	25.00±0.01	25.5±0.5	150.0±2.0	159±1	1.06±0.02	0.0406±0.0006	99.94
KL 240806-5	25.00±0.01	25.5±0.5	150.0±2.0	439±2	2.92±0.04	0.132±0.002	99.56
KL 240806-6	25.00±0.01	25.5±0.5	150.0±2.0	221±1	1.48±0.02	0.0732±0.0009	99.97
KL 240807-1	25.00±0.01	25.5±0.5	150.0±2.0	560±2	3.74±0.05	0.172±0.001	99.98
KL 240807-2	8.50±0.01	10.1±0.5	150.0±2.0	588±3	3.92±0.05	0.0706±0.0002	99.99
KL 240807-4	8.50±0.01	10.1±0.5	150.0±2.0	471±2	3.14±0.04	0.0557±0.0003	99.99
KL 240807-5	8.50±0.01	10.1±0.5	150.0±2.0	296±2	1.97±0.03	0.03519±0.00006	99.99
KL 240808-1	8.50±0.01	10.1±0.5	150.0±2.0	354±2	2.36±0.03	0.0424±0.0004	99.98
KL 240808-2	8.50±0.01	10.1±0.5	150.0±2.0	179±1	1.19±0.02	0.01977±0.00008	99.98
KL 240808-3	8.50±0.01	10.1±0.5	150.0±2.0	238±2	1.58±0.02	0.0259±0.0001	99.99
KL 240808-4	8.50±0.01	10.1±0.5	150.0±2.0	121±1	0.81±0.01	0.01024±0.00008	99.93
KL 240808-5	8.50±0.01	10.1±0.5	150.0±2.0	414±2	2.76±0.04	0.0455±0.0001	99.98
KL 240809-1	8.50±0.01	10.1±0.5	150.0±2.0	62±1	0.42±0.01	0.00756±0.00007	99.95
KL 240809-2	8.50±0.01	10.1±0.5	150.0±2.0	532±2	3.55±0.05	0.0582±0.0003	99.98
KL 240809-3	20.00±0.01	20.7±0.5	150.0±2.0	615±3	4.10±0.06	0.131±0.001	99.96
KL 240809-4	20.00±0.01	20.7±0.5	150.0±2.0	126±1	0.84±0.01	0.0152±0.0004	99.67
KL 240809-6	20.00±0.01	20.7±0.5	150.0±2.0	65±1	0.44±0.01	0.01186±0.00006	99.98
KL 240812-1	20.00±0.01	20.7±0.5	150.0±2.0	374±2	2.50±0.04	0.0783±0.0005	99.98
KL 240812-2	20.00±0.01	20.7±0.5	150.0±2.0	189±1	1.26±0.02	0.0410±0.0002	99.99

Table S2 (continued). Overview of experimental conditions for IPN in DI water. Uncertainties are at the ±1σ level.

Internal reference	$T_{setpoint}$ (°C)	$T_{corrected}$ (°C)	V_l (mL)	Φ (mL min^{-1})	$\frac{\Phi}{V_l}$ (min^{-1})	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min^{-1})	r (%)
KL 240812-3	20.00±0.01	20.7±0.5	150.0±2.0	560±2	3.74±0.05	0.112±0.001	99.98
KL 240812-4	20.00±0.01	20.7±0.5	150.0±2.0	314±2	2.09±0.03	0.0657±0.0005	99.98
KL 240812-5	20.00±0.01	20.7±0.5	150.0±2.0	437±2	2.91±0.04	0.0905±0.0004	99.98
KE 250704-1	25.00±0.01	25.5±0.5	100.0±2.0	253±1	2.53±0.05	0.102±0.004	99.76
KE 250704-2	25.00±0.01	25.5±0.5	100.0±2.0	378±2	3.78±0.08	0.16±0.01	99.68
KE 250704-3	25.00±0.01	25.5±0.5	100.0±2.0	65±1	0.65±0.02	0.0284±0.0006	99.78
KE 250707-1	25.00±0.01	25.5±0.5	100.0±2.0	503±2	5.03±0.10	0.23±0.01	99.89
KE 250707-2	25.00±0.01	25.5±0.5	100.0±2.0	160±1	1.60±0.03	0.069±0.002	99.83
KE 250708-1	20.00±0.01	20.7±0.5	100.0±2.0	374±2	3.74±0.08	0.114±0.008	99.55
KE 250708-2	20.00±0.01	20.7±0.5	100.0±2.0	250±1	2.50±0.05	0.066±0.004	99.56
KE 250708-3	20.00±0.01	20.7±0.5	100.0±2.0	65±1	0.65±0.02	0.0209±0.0003	99.83
KE 250709-1	20.00±0.01	20.7±0.5	100.0±2.0	498±2	4.98±0.10	0.16±0.01	99.68
KE 250709-2	20.00±0.01	20.7±0.5	100.0±2.0	157±1	1.57±0.03	0.050±0.002	99.58

Table S3. Overview of experimental conditions for IBN in DI water. Uncertainties are at the ±1σ level.

Internal reference	$T_{setpoint}$ (°C)	$T_{corrected}$ (°C)	V_l (mL)	Φ (mL min^{-1})	$\frac{\Phi}{V_l}$ (min^{-1})	$\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min^{-1})	r (%)
~~KE 250714-1~~*	~~20.00±0.01~~	~~20.7±0.5~~	~~100.0±2.0~~	~~248±1~~	~~2.48±0.05~~	~~0.154±0.008~~	~~99.47~~
KE 250714-2	20.00±0.01	20.7±0.5	100.0±2.0	95±1	0.95±0.02	0.047±0.001	99.89
KE 250714-5	20.00±0.01	20.7±0.5	100.0±2.0	64±1	0.64±0.01	0.0321±0.0006	99.88
KE 250715-1	20.00±0.01	20.7±0.5	100.0±2.0	204±1	2.04±0.04	0.10±0.01	98.78
KE 250715-2	20.00±0.01	20.7±0.5	100.0±2.0	143±1	1.43±0.03	0.071±0.003	99.83
KE 250715-3	20.00±0.01	20.7±0.5	100.0±2.0	46±1	0.46±0.01	0.02521±0.00007	100.0

* not used in the analysis.

Table S4. Linear regression analyses of d/dt(ln(A_0/A_t) versus Φ/V_l for the data shown in Figures 3 and S2. Uncertainties are at the ±1σ level.

Compound	Solvent	T (K)	Slope	Intercept (min^{-1})	r (%)
IPN	n-octanol	284.65	$(0.65\pm0.02)\times10^{-3}$	$(1.0\pm0.8)\times10^{-4}$	99.76
		293.85	$(1.03\pm0.04)\times10^{-3}$	$-(0.6\pm1.3)\times10^{-4}$	99.37
		298.65	$(1.16\pm0.02)\times10^{-3}$	$(0.7\pm0.6)\times10^{-4}$	99.86
		304.95	$(1.42\pm0.09)\times10^{-3}$	$(4.0\pm3.0)\times10^{-4}$	98.57
		309.65	$(2.16\pm0.14)\times10^{-3}$	$(0.4\pm5.2)\times10^{-4}$	98.72
IBN	n-octanol	284.65	$(2.05\pm0.14)\times10^{-4}$	$(0.8\pm0.5)\times10^{-4}$	99.04
		293.85	$(3.67\pm0.07)\times10^{-4}$	$-(0.3\pm0.2)\times10^{-4}$	99.83
		298.65	$(4.14\pm0.20)\times10^{-4}$	$-(0.3\pm0.2)\times10^{-4}$	98.93
		304.95	$(6.25\pm0.61)\times10^{-4}$	$-(0.2\pm2.1)\times10^{-4}$	96.40
		309.65	$(7.76\pm0.30)\times10^{-4}$	$(2.3\pm1.1)\times10^{-4}$	99.54
IPN	DI water	283.25	$(1.78\pm0.06)\times10^{-2}$	$-(1.6\pm1.5)\times10^{-3}$	99.51
		293.85	$(3.17\pm0.10)\times10^{-2}$	$-(3.1\pm2.8)\times10^{-3}$	99.46
		298.25	$(4.42\pm0.12)\times10^{-2}$	$-(1.1\pm2.9)\times10^{-3}$	99.42
IBN	DI water	293.25	$(4.74\pm0.08)\times10^{-2}$	$(2.6\pm1.0)\times10^{-3}$	99.96

70

Table S5. Dimensionless Henry's law constants of EN, IPN, and IBN. Uncertainties are at the ±1σ level. n/d = not determined.

		H_S^{cc} (unitless)					
Compound	***T*** **(K) / Reference**	**283.25**	**284.65**	**293.85**	**298.65**	**304.95**	**309.65**
EN in n-octanol	[1]	896±200 (281.7 K)	n/d	535±30 (293.2 K)	378±37 (298.2 K)	n/d	n/d
IPN in n-octanol	This work	n/d	1547±53	972±36	864±13	706±43	463±30
IBN in n-octanol	This work	n/d	4869±339	2726±50	2417±119	1599±156	1289±50
EN in DI water	[1]	91.9±1.1 (281.7 K)	n/d	48.8±1.5 (293.2 K)	38.0±0.7 (298.2 K)	n/d	n/d
IPN in DI water	This work	56.0±2.0	n/d	31.5±1.0	22.6±0.6	n/d	n/d
IBN in DI water	This work	n/d	n/d	21.1±0.4	n/d	n/d	n/d

Table S6. Liquid-phase loss rate constants of EN, IPN and IBN. Uncertainties are at the ±1σ level. n/d = not determined.

		k_1 (10^{-5} s^{-1})					
Compound	***T*** **(K) / Reference**	**283.25**	**284.65**	**293.85**	**298.65**	**304.95**	**309.65**
EN in n-octanol	[1]	0.8±1.9 (281.7 K)	n/d	-0.9±1.3 (293.2 K)	-4.7±2.3 (298.2 K)	n/d	n/d
IPN in n-octanol	This work	n/d	0.17±0.13	-0.10±0.21	0.11±0.09	0.67±0.50	0.07±0.86
IBN in n-octanol	This work	n/d	0.13±0.08	-0.06±0.04	0.13±0.11	-0.04±0.36	0.39±0.18
EN in DI water	[1]	0.4±0.6 (281.7 K)	n/d	0.1±3.8 (293.2 K)	5.8±2.2 (298.2 K)	n/d	n/d
IPN in DI water	This work	-2.7±2.6	n/d	-5.2±4.6	-1.8±4.9	n/d	n/d
IBN in DI water	This work	n/d	n/d	4.3±1.7	n/d	n/d	n/d

References

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