

Supplementary Materials

Table 1. Data used for computation of solvent solubility parameters (δ_2).

Solvent	δ_2	Data from [9]				Data from [12]	
		δ_d	δ_p	δ_h	V_2	V_2	T
Acetic acid	21.37	14.5	8.0	13.5	57.6	57.5	25
Acetone	19.94	15.5	10.4	7.0	73.8	74.0	25
Acetonitrile	24.40	15.3	18.0	6.1	52.9	52.2	20
Benzene	18.51	18.4	0.0	2.0	89.5	89.1	20
n-Butyl acetate	17.41	15.8	3.7	6.3	132.6	131.6	20
Cyclohexane	16.80	16.8	0.0	0.2	108.9	108.7	25
Diethyl ether	15.49	14.5	2.9	4.6	104.7	103.8	20
Ethanol	26.52	15.8	8.8	19.4	58.6	58.4	20
Ethyl acetate	18.15	15.8	5.3	7.2	98.6	97.9	20
Ethylene glycol	32.95	17.0	11.0	26.0	55.9	55.7	20
Heptane	15.30	15.3	0.0	0.0	147.0	147.5	20
n-Hexane	14.90	14.9	0.0	0.0	131.4	130.4	25
Methanol	29.41	14.7	12.3	22.3	40.6	40.5	20
Methyl hydroperoxide *	29.40	14.9	13.1	21,7	48.9	48.9	20
1-propanol	24.60	16.0	6.8	17,4	75.1	75.1	25
Pentane	14.50	14.5	0.0	0,0	116.0	115.2	20
Propan-2-ol	23.58	15.8	6.1	16,4	76.9	77.0	25
Tetrahydrofuran	19.46	16.8	5.7	8,0	81.9	81.6	25
Toluene	18.16	18.0	1.4	2,0	106.6	106.9	25
Xylene	18.10	17.8	1.0	3,1	121.1	121.3	25

Total solubility parameters δ_2 were calculated using the HSP values from [9]. Molar volumes V_2 (cm^3/mol) quoted in [9] were checked against values that were calculated from density at T ($^\circ\text{C}$) and molecular weight as in [12]. * : HSPs of methyl hydroperoxide were calculated using the software HSPiP and V_2 from [20,21]. All solubility parameters are given in $(\text{MPa})^{0.5}$.

Table S2. Expressions used for the calculation of the solubility maximum-minimum ratio.

Variable	Uncertainty absolute	Expression for calculation of span ratio $R = \max(x_1)/\min(x_1)$
ΔH_1	± 5 kJ/mol	$\exp(2 \cdot \Delta(\Delta H_1) \cdot 1/R \cdot (1/T - 1/T_{m,1}))$
$T_{m,1}$	± 5 K	$\exp(2 \cdot \Delta H_1/R \cdot \Delta T \cdot (T_{m,1}^2 - \Delta T ^2)^{-1})$
V_1	± 4 cm ³ /mol	$\exp(2 \cdot 1/RT \cdot \Delta V_1 \cdot (\Delta\delta)^2)$
δ_1	± 1 (MPa) ^{0.5}	$\exp(4 \cdot V_1/RT \cdot \Delta\delta \cdot \Delta\delta_1)$
δ_2	± 1 (MPa) ^{0.5}	$\exp(4 \cdot V_1/RT \cdot \Delta\delta \cdot \Delta\delta_2)$

The span ratio R rates the influence a variable has on the solubility x_1 as calculated from Equation 1 and, resp., Equation 2. The uncertainties of the variables quoted above were derived from literature data. Taking the absolute value of the uncertainty of a variable, for instance, $|\Delta V_1| = 4$ cm³/mol and putting it into the respective equation gives the span ratio with respect to the variable V_1 .

Table S3. Experimental and calculated mole fraction solubilities x_1 of L-ascorbic acid.

Solvent	δ_2	Experimental x_1				Calculated x_1
		T=293.15 [36]	T=293 [34]	T=298.15 [35]	T=298 [34]	T=298 this study
Acetone	19.94	-	0.00026	-	0.00032	6.80E-08
Acetonitrile	24.40	-	0.00020	-	0.00024	2.32E-05
Ethanol	26.52	0.00531	0.00229	0.00375	0.00274	7.76E-05
Ethyl acetate	18.15	-	0.00010	-	0.00013	5.24E-09
Methanol	29.41	0.01629	0.01006	-	0.01083	5.03E-04
1-propanol	24.60	-	-	0.00218	-	1.48E-05
Propan-2-ol	23.58	0.00222	0.00051	-	0.00063	5.35E-06
Tetrahydrofuran	19.46	-	0.00053	-	0.00067	3.53E-08

Total solubility parameters δ_2 were calculated using the HSP component values from [9]. All solubility parameters are given in (MPa)^{0.5}. Temperatures are given in degree Kelvin.