

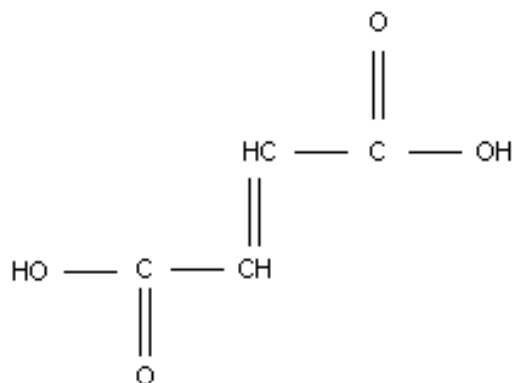
PHYSICAL and CHEMICAL PROPERTIES:

FUMARIC ACID

Chemical Name *trans*-Butenedioic acid

Molecular Formula C₄H₄O₄

Structural Formula



Appearance White crystals

Odour None

Taste Tart

Molecular Weight 116.07

Acid Equivalent Weight 58.04

Specific Gravity (20°C/4°C) 1.635

Melting Point (°C) 286

Flash Point (°C)
(Cleveland Open Cup) 282

Solubility in Water

Temp (°C)	Temp (°F)	Solubility* (%w/w)	Temp (°C)	Temp (°F)	Solubility* (%w/w)
5	41	0.28	45	113	1.31
10	50	0.34	50	122	1.58
15	59	0.41	55	131	1.92
20	68	0.50	60	140	2.33
25	77	0.61	65	149	2.82
30	86	0.73	70	158	3.42
35	95	0.89	75	167	4.15
40	104	1.08	80	176	5.03

*calculated using the following equation from: Lange N.A. & Sinks M.H. 1930. The solubility, specific gravity and index of refraction of aqueous solutions of fumaric, maleic and *i*-malic acids. *J. Am. Chem. Soc.* 52: 2602-2604

$$\log(C) = 0.01672(t) - 0.6362,$$

where C = %w/w acid concentration and t = temperature (°C)

Solubility of Calcium Salt (as the trihydrate)	1.22 %w/w at 20°C
Solubility of Sodium Salt	22 %w/v at 20°C
Solubility in 95% Ethanol	5.44 %w/w at 30°C
Log(octanol/water partition coefficient)	0.25
Log(ether/water partition coefficient)	0.07

Dissociation Constants at 25°C vs. Ionic Strength, I

	$I = 0$	$I = 0.005$	$I = 0.05$	$I = 0.10$
pK_{a1} :	3.05*	2.98**	2.88**	2.85*
pK_{a2} :	4.49*	4.36**	4.14**	4.10*

*from Smith, W. & Martell, A.E. 1989. *Critical Stability Constants*, vol. 6, second supplement. Plenum Press, New York.

**calculated using the equations of Butler, J.N. 1998. *Ionic Equilibrium: Solubility and pH Calculations*. John Wiley & Sons, Inc., New York.

Acid Strength, (defined as the % w/v of acid required to lower the pH of 0.005N NaOH solution to a specific value*)

↓ Acid ↓	pH ⇒	2.5	3.0	3.5	4.0	4.5	5.0	5.5
Citric, anhydrous		0.717	0.239	0.128	0.090	0.069	0.055	0.047
Citric, monohydrate		0.784	0.262	0.140	0.098	0.075	0.060	0.051
Fumaric		0.372	0.128	0.070	0.048	0.037	0.032	0.030
Lactic, 80%		1.884	0.484	0.177	0.093	0.068	0.060	0.057
Malic		0.953	0.273	0.121	0.076	0.057	0.045	0.038
Phosphoric, 85%		0.130	0.077	0.064	0.059	0.058	0.057	0.056
Sodium Acid Sulfate, 93%		0.133	0.084	0.070	0.066	0.065	0.065	0.065
L-Tartaric		0.469	0.161	0.086	0.059	0.046	0.041	0.039
↑ Acid ↑	pH ⇒	2.5	3.0	3.5	4.0	4.5	5.0	5.5

*for diprotic acids, calculated using the following equation:

$$\begin{aligned} \text{\%w/v of acid required to} \\ \text{lower the pH of NaOH} \\ \text{solution to a specific} \\ \text{value} \end{aligned} = \frac{([\text{Na}^+] + [\text{H}^+]) (\text{mol.wt.}) (0.1)}{\frac{2K_{a1}K_{a2}}{[\text{H}^+]^2 + K_{a1}[\text{H}^+] + K_{a1}K_{a2}} + \frac{K_{a1}[\text{H}^+]}{[\text{H}^+]^2 + K_{a1}[\text{H}^+] + K_{a1}K_{a2}}}$$