

Inorganic acids	CAS number	EHS	Clean chemistry	Greenness	pKa <sup>a</sup>	GRAS <sup>b</sup>	Comment
Hydrochloric acid	7647-01-0	7	7	7.3	-8	YES	Waste disposal issues upon incineration. Halogenated waste.
Hydrobromic acid	10035-10-6	7	7	7.3	-9	NO	Waste disposal issues upon incineration. Halogenated waste.
Phosphoric acid, dilute	7664-38-2	7	7	7.3	1.90, 6.74, 11.74	YES	Waste disposal issues upon incineration.
Sulfuric acid, dilute	7664-93-9	7	7	7.3	-3.19, 1.98	NO	Waste disposal issues upon incineration.
Hydroiodic acid	10034-85-2	7	5	6.4	-9.9	NO	Causes severe burns (R35). Waste disposal issues upon incineration. Halogenated waste. Purple plumes of iodine.
Phosphoric acid	7664-38-2	7	5	6.4	1.90, 6.74, 1.74	YES	Waste disposal issues upon incineration.
Sulfuric acid	7664-93-9	7	5	6.4	-3.19, 1.98	NO	Causes severe burns (R35). Waste disposal issues upon incineration.
Nitric acid	7697-37-2	5	3	4.3	-1.37	NO	Strong oxidant (R8). Causes severe burns (R35).
Hydrogen fluoride	7664-39-3	3	5	4.2	3.2	NO	Toxic (R26/27/28). Causes severe burns (R35). Special vessel necessary. Waste disposal issues upon incineration. Halogenated waste.
Perchloric acid	7601-90-3	3	3	3.0	~5	NO	Strong oxidant (R8). Causes severe burns (R35). Waste disposal issues upon incineration. Halogenated waste.
Organic acids	CAS number	EHS	Clean chemistry	Greenness	pKa <sup>a</sup>	GRAS <sup>b</sup>	Comment
Glutaric acid	110-94-1	10	9	9.3	4.41, 5.52	NO	
Citric acid	77-92-9	10	7	8.5	2.93	YES	
Ascorbic acid	50-81-7	10	7	8.5	4.09	YES	
p-TsOH (monohydrate)	6192-52-5	10	7	8.5	-6.57	NO	
Benzoic acid	65-85-0	7	9	8.0	4.20	YES	
Oxalic acid	144-62-7	7	9	8.0	1.25, 4.23	NO	
Pivalic acid	75-98-9	7	9	8.0	4.94	NO	
Succinic acid	110-15-6	7	9	8.0	4.24	YES	
Acetic acid	64-19-7	7	9	7.5	4.76	YES	Causes severe burns (R35).
Propionic acid	79-09-4	7	9	7.5	4.79	YES	
Formic acid, dilute	64-18-6	7	9	7.5	3.75	YES	
Methanesulfonic acid	75-75-2	7	7	7.3	-1.92	NO	
Formic acid	64-18-6	7	7	6.9	3.75	YES	Causes severe burns (R35).
Trifluoromethanesulfonic acid	1493-13-6	7	5	6.1	-12	NO	Causes severe burns (R35). Waste disposal issues upon incineration. Halogenated waste.
Trifluoroacetic acid	76-05-1	7	5	6.0	0.50	NO	Causes severe burns (R35). Waste disposal issues upon incineration. Halogenated waste.
Trichloroacetic acid	76-03-9	3	5	3.6	0.52	NO	Causes severe burns (R35). Waste disposal issues upon incineration. Halogenated waste.

<sup>a</sup> When available, literature pKa data was obtained from measurements taken at 25 °C and at ionic strength approaching 0. Numbers in italics are not experimentally obtained data.

<sup>b</sup> GRAS (Generally Recognized as Safe) is an FDA designation that a chemical or substance added to food is considered safe by experts.

<http://www.fda.gov/food/ingredientspackaginglabeling/gras/default.htm>

Carbonates	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Sodium bicarbonate	144-55-8	10	9	9.3	5.95	YES	
Potassium bicarbonate	298-14-6	10	9	9.3	5.95	YES	
Sodium carbonate	497-19-8	10	9	9.3	9.1	YES	
Potassium carbonate	584-08-7	9	9	8.8	9.1	NO	
Cesium carbonate	534-17-8	10	5	7.4	9.1	NO	
Phosphates	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Trisodium phosphate	7601-54-9	10	7	8.2	11.74	YES	Waste disposal issues upon incineration.
Tripotassium phosphate	7778-53-2	7	6	6.7	11.74	YES	Waste disposal issues upon incineration.
Hydroxides	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Potassium hydroxide	1310-58-3	7	9	8.0	15.74	YES	Causes severe burns (R35).
Sodium hydroxide	1310-73-2	7	9	8.0	15.74	YES	Causes severe burns (R35).
Calcium hydroxide	1305-62-0	7	9	8.0	15.74	YES	
Barium hydroxide	17194-00-2	7	8	7.7	15.74	NO	
Lithium hydroxide	1310-65-2	4	8	5.7	15.74	NO	
Hydrides	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Sodium hydride	7646-69-7	5	5	5.0	35.0	NO	May cause runaway reaction with certain solvents, such as DMF, DMA. Highly flammable gaseous by-product (hydrogen) needs abating. Use of mineral oil dispersions greatly reduce fire hazard.
Potassium hydride	7693-26-7	5	5	5.0	35.0	NO	May cause runaway reaction with certain solvents, such as DMF, DMA. Highly flammable gaseous by-product (hydrogen) needs abating. Use of mineral oil dispersions greatly reduce fire hazard.
Acetates	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Potassium acetate	127-08-2	10	9	9.3	4.76	NO	
Sodium acetate	127-09-3	10	9	9.3	4.76	YES	
Alkoxides	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Sodium methoxide	124-41-4	5	9	6.9	15.1	NO	Highly flammable (R11). Toxic (R23/24/25).
Sodium ethoxide	141-52-6	5	9	6.6	15.93	NO	Highly flammable (R11).
Sodium <i>tert</i> -butoxide	865-48-5	5	9	6.9	19.2	NO	Highly flammable (R11). Causes severe burns (R35).
Potassium <i>tert</i> -butoxide	865-47-4	5	9	6.9	19.2	NO	Highly flammable (R11). Causes severe burns (R35).
Lithium methoxide	865-34-9	4	8	5.7	15.1	NO	Highly flammable (R11). Toxic (R23/24/25).
Lithium ethoxide	2388-07-0	4	8	5.7	15.93	NO	Highly flammable (R11).
Lithium <i>tert</i> -butoxide	1907-33-1	4	8	5.7	19.2	NO	Highly flammable (R11).

Phosphazanes	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
Phosphazane BEMP	98015-45-3	7	5	6.0	27.58	NO	
Phosphazane P2-Et	165535-45-5	7	5	6.0	32.66	NO	
Amines	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
2-Methylpyridine	109-06-8	8	9	8.3	5.97	NO	
2,6-Lutidine	108-48-5	8	9	8.3	6.75	NO	
DBN	3001-72-7	7	9	8.0	13.5	NO	
Pyridine	110-86-1	7	9	7.5	5.17	NO	Highly flammable (R11).
4-Methylpyridine	108-89-4	7	9	7.5	6.02	NO	Toxic (R24).
Morpholine	110-91-8	7	9	7.5	8.49	NO	
Diethylaminopropylamine	104-78-9	7	9	7.5	10.48	NO	
Tetramethylguanidine	80-70-6	7	9	7.5	13.6	NO	
DBU	6674-22-2	7	8	7.3	12.5	NO	Causes severe burns (R35).
2,2,6,6-Tetramethylpiperidine	768-66-1	7	8	7.3	11.1	NO	
Triethylamine	121-44-8	5	9	6.9	10.77	NO	Highly flammable (R11). Toxic (R23/24). Causes severe burns (R35).
Diisopropylamine	108-18-9	5	9	6.9	11.05	NO	Highly flammable (R11).
Piperidine	110-89-4	5	9	6.9	11.22	NO	Highly flammable (R11). Toxic (R23/24).
Dimethylethylamine	598-56-1	5	9	6.9	10.16	NO	Highly flammable (R11).
Dipropylamine	142-84-7	5	9	6.9	10.91	NO	Highly flammable (R11). Causes severe burns (R35).
N-Methylmorpholine	109-02-4	5	9	6.9	7.41	NO	Highly flammable (R11).
n-Butylamine	109-73-9	5	9	6.9	10.61	NO	Highly flammable (R11). Causes severe burns (R35).
Diethylamine	109-89-7	5	9	6.9	10.98	NO	Highly flammable (R11). Causes severe burns (R35).
Ammonia	7664-41-7	5	9	6.5	9.21	NO	Toxic (R23).
Diisopropylethylamine	7087-68-5	5	9	6.5	10.75	NO	Highly flammable (R11).
tert-Butylamine	75-64-9	5	9	6.5	10.63	NO	Highly flammable (R11). Toxic (R25). Causes severe burns (R35).
DABCO®	280-57-9	5	9	6.5	8.4	NO	Highly flammable (R11).
Cyclohexylamine	108-91-8	5	9	6.5	10.62	NO	
Tributylamine	102-82-9	5	7	6.3	9.93	NO	Toxic (R23/24/25).
4-(Dimethylamino)pyridine	1122-58-3	3	9	5.2	9.60	NO	Toxic (R25/27).
Dicyclohexylamine	101-83-7	3	7	4.3	11.25	NO	Toxic (R24/25).
Imidazole	288-32-4	2	9	3.9	6.99	NO	Toxic (R61).

Disilazides	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
KHMDS	40949-94-8	5	7	5.9	29.5	NO	Highly flammable (R11).
NaHMDS	1070-89-9	5	7	5.9	29.5	NO	Highly flammable (R11).
LiHMDS	4039-32-1	4	8	5.5	29.5	NO	Highly flammable (R11).
Amides	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
LiTMP	38227-87-1	4	8	5.5	37.3	NO	.
LDA	4111-54-0	3	8	4.5	35.7	NO	Highly flammable (R11).
Sodium amide	7782-92-5	4	3	3.7	35.0	NO	Forms peroxide. Toxic and flammable gaseous by-product (ammonia) needs abating.
Lithium amide	7782-89-0	4	3	3.7	35.0	NO	Forms peroxide. Toxic and flammable gaseous by-product (ammonia) needs abating.
Alkyllithiums	CAS number	EHS	Clean Chemistry	Greenness	pKa <sup>a</sup> (BH <sup>+</sup> )	GRAS <sup>b</sup>	Comment
<i>n</i> -Hexyllithium	21369-64-2	2	8	4.0	40.0	NO	Highly flammable (R11). Causes severe burns (R35).
<i>n</i> -Butyllithium	109-72-8	1	7	3.1	50.0	NO	Highly flammable (R11). Highly flammable gaseous by-product (butane) needs abating.
<i>sec</i> -Butyllithium	598-30-1	1	7	3.1	51.0	NO	Highly flammable (R11). Causes severe burns (R35). Highly flammable gaseous by-product (butane) needs abating.
<i>tert</i> -Butyllithium	594-19-4	1	7	3.1	53.0	NO	Highly flammable (R11). Highly flammable gaseous by-product (butane) needs abating.

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