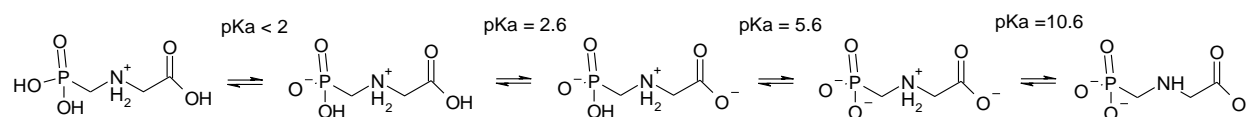


## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

Glyphosate is an organic acid composed of a phosphonomethyl and glycine component. The chemical name for glyphosate is *N*-(phosphonomethyl) glycine. Glyphosate is a zwitterion with four distinct dissociation constants ( $pK_a$  values are depicted below) and exists as different ionic species depending on the pH of its surroundings. Glyphosate is an amphoteric chemical and may react as an acid or a base under certain conditions.



Glyphosate isopropylamine (Chemical Abstracts Registry Number [CASRN] 38641-94-0) is one of the salt forms of glyphosate used in commercial herbicides employing glyphosate as an active ingredient. This substance is registered as a pesticide by the EPA (1993) and is used to control broadleaf weeds and grasses; in food and nonfood settings, flower gardens, lawns, turf, residential areas, and forests; and along roadsides. Use of glyphosate as a pesticide outside of an agricultural context would be considered non-agricultural. Some labels may list the active ingredient in a formulation of glyphosate and the acid equivalents (AE), which is the theoretical yield of the parent acid from the formulated ester or salt. For example, the AE of glyphosate isopropylamine salts is 74%.

Detailed information on the chemical identity of glyphosate and glyphosate isopropylamine is provided in Table 4-1.

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Detailed information on the physical and chemical properties of glyphosate and glyphosate isopropylammonium is provided in Table 4-2.

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of Glyphosate and Glyphosate Isopropylamine<sup>a</sup>**

Characteristic	Information	
Chemical name	Glyphosate	Glyphosate isopropylamine
Synonym(s)	Glyphosphate; N-(phosphonomethyl) glycine; phosphonomethyliminoacetic acid; glyphosate acid	Glycine, N-(phosphonomethyl)-, compound with 2-propanamine (1:1); glyphosate-isopropylammonium; glyphosate mono(isopropylamine) salt; glyphosate-mono(isopropylammonium); N-(phosphonomethyl)glycine, isopropylamine salt
Partial list of registered trade name(s)	Pondmaster; Roundup® Max; Glifoglex; Glycel; Muster; Rondo; Sonic; Spasor; Sting; Tumbleweed; MON-0573; CP 67573	Roundup®; Rondo; Rodeo; Glifonox; Glycel; MON-0139; CP 70139; Shackle <sup>b</sup>
Chemical formula	C <sub>3</sub> H <sub>8</sub> NO <sub>5</sub> P	C <sub>3</sub> H <sub>8</sub> NO <sub>5</sub> P.C <sub>3</sub> H <sub>9</sub> N
Chemical structure		
CAS Registry Number	1071-83-6	38641-94-0

<sup>a</sup>All information obtained from McBean (2011), O'Neil et al. (2013), and/or ChemIDplus (2017) unless noted otherwise.

<sup>b</sup>EPA 1993.

CAS = Chemical Abstracts Service

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Glyphosate and its Isopropylamine Salt<sup>a</sup>**

Property	Glyphosate	Glyphosate isopropylamine salt
Molecular weight	169.1	228.2
Color	White	White
Physical state	Solid; crystals	Powder
Melting point	230°C (decomposes)	Two stages: 143–164 and 189–223°C
Boiling point	No data	Decomposes without boiling
Density at 20°C	1.705	1.482
Odor	Odorless	Odorless
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25°C	12,000 mg/L 10,500 mg/L (pH 1.9, 20°C)	1,050,000 mg/L (pH 4.3, 25°C)
Organic solvent(s)	Insoluble in most organic solvents: acetone, ethanol, and xylene	Dichloromethane 184 mg/L at 20°C; methanol 15,880 mg/L at 20°C
Dissociation constants:	pKa <sub>1</sub> 0.8; pKa <sub>2</sub> 3; pKa <sub>3</sub> 6; pKa <sub>4</sub> 11; pKa <sub>1</sub> <sup>b</sup> <2; pKa <sub>2</sub> <sup>b</sup> 2.6; pKa <sub>3</sub> <sup>b</sup> 5.6; pKa <sub>4</sub> <sup>b</sup> 10.6	pKa <sub>1</sub> 2.18 at 20°C (monophosphate); pKa <sub>2</sub> 5.77 at 20°C (carboxylic acid)
Partition coefficients:		
Log K <sub>ow</sub>	<-3.4	-5.4
Log K <sub>oc</sub>	3.4–3.7 (K <sub>oc</sub> =2,600–4,900) <sup>c</sup> -2.8–3.1 (K <sub>oc</sub> =0.00169–2,080 L/kg) <sup>d</sup>	3.3 (K <sub>oc</sub> = 2,080 L/kg) <sup>d</sup>
Vapor pressure at 25°C	9.8x10 <sup>-8</sup> mmHg	1.58x10 <sup>-8</sup> mmHg
Henry's law constant	2.1x10 <sup>-12</sup> atm-m <sup>3</sup> /mol at 25°C <sup>d</sup>	3.3x10 <sup>-15</sup> atm-m <sup>3</sup> /mol at 25°C <sup>e</sup>
Autoignition temperature	No data	No data
Flashpoint	Not flammable	No data
Flammability limits	No data	No data
Explosive limits	No data	No data

<sup>a</sup>All information obtained from either McBean (2011) or O'Neil et al. (2013).

<sup>b</sup>Sprinkle et al. 1975.

<sup>c</sup>Glass 1987.

<sup>d</sup>Predicted values from EPA CompTox Chemicals Dashboard

<sup>e</sup>EPI Suite 2012.