Name:	Acid Yellow 3
CAS:	8004-92-0
Transport:	25kgs
Melting Point:	150 C (Decomposes)
Stability:	Stable at room temperature in closed containers under normal storage and handling conditions.
Solubility:	Souluble (40g/l) SOLVENT MEG (25), DEG (55), Isopropanol (150), PG (35), G
Appearance:	yellow to orange powder
Specification:	The C.I. Acid Yellow 3, with the cas register number 8004-92-0, has its IUPAC name of disodium 2-(1,3-dioxoinden-2-yl)quinoline-6,8-disulfonate. This is a kind of yellow to orange-brown powder and is soluble in water and slightly soluble in ethanol. It belongs to the product category of Quinolinecarboxylic Acids, etc. The characteristics of this chemical are as below: (1)H-Bond Acceptor: 9; (2)Rotatable Bond Count: 1; (3)Tautomer Count: 3; (4)Exact Mass: 476.956497; (5)MonoIsotopic Mass: 476.956497; (6)Topological Polar Surface Area: 178; (7)Heavy Atom Count: 31; (8)Complexity: 853; (9)Covalently-Bonded Unit Count: 3. You should be cautious while dealing with this chemical. This is a kind of harmful chemical which may cause damage to health. If swallowed, it will be very harmful. Besides, it is irritant to eyes, respiratory system and skin, and it may cause inflammation to the skin or other mucous membranes. So while using it, we should be very cautious. Wear suitable protective clothing and avoid contacting with skin and eyes. If in case of contacting with eyes, rinse immediately with plenty of water and seek medical advice. The following datas could be converted into the molecular structure: (1)Canonical SMILES: C1=CC=C2C(=C1)C(=O)C(C2=O)C3=NC4=C(C=C(C=C4C=C3)S(=O)(=O)[O-])S(=O)(=O) [O-].[Na+].[Na+]

(2)InChI: InChI=1S/C18H11NO8S2.2Na/c20-17-11-3-1-2-4-12(11)18(21)15(17)13-6-5-9-7-10(28(22,23)24)8-14(16(9)19-13)29(25,26)27;;/h1-8,15H,(H,22,23,24)(H,25,26,27);;/q;2*+1/p-2

(3)InChIKey: FZUOVNMHEAPVBW-UHFFFAOYSA-L

Below are the toxicity information which have been tested:

Organism	Test Type	Route	Reported Dose (Normalized Dose)	Effect	Source
rat	LD50	oral	2gm/kg (2000mg/kg)		Scientia Pharmaceutica. Vol. 47, Pg. 39, 1979.

Report:

The C.I. Acid Yellow 3, with the cas register number 8004-92-0, has its IUPAC name of disodium 2-(1,3-dioxoinden-2-yl)quinoline-6,8-disulfonate. This is a kind of yellow to orange-brown powder and is soluble in water and slightly soluble in ethanol. It belongs to the product category of Quinolinecarboxylic Acids, etc.

The characteristics of this chemical are as below: (1)H-Bond Acceptor: 9; (2)Rotatable Bond Count: 1; (3)Tautomer Count: 3; (4)Exact Mass: 476.956497; (5)MonoIsotopic Mass: 476.956497; (6)Topological Polar Surface Area: 178; (7)Heavy Atom Count: 31; (8)Complexity: 853; (9)Covalently-Bonded Unit Count: 3.

You should be cautious while dealing with this chemical. This is a kind of harmful chemical which may cause damage to health. If swallowed, it will be very harmful. Besides, it is irritant to eyes, respiratory system and skin, and it may cause inflammation to the skin or other mucous membranes. So while using it, we should be very cautious. Wear suitable protective clothing and avoid contacting with skin and eyes. If in case of contacting with eyes, rinse immediately with plenty of water and seek medical advice.

The following datas could be converted into the molecular structure:

(1)Canonical SMILES: C1=CC=C2C(=C1)C(=O)C(C2=O)C3=NC4=C(C=C(C=C4C=C3)S(=O)(=O)[O-])S(=O)(=O) [O-].[Na+].[Na+]

(2)InChI: InChI=1S/C18H11NO8S2.2Na/c20-17-11-3-1-2-4-12(11)18(21)15(17)13-6-5-9-7-10(28(22,23)24)8-14(16(9)19-13)29(25,26)27;;/h1-8,15H,(H,22,23,24)(H,25,26,27);;/q;2*+1/p-2

(3)InChIKey: FZUOVNMHEAPVBW-UHFFFAOYSA-L

Below are the toxicity information which have been tested:

Organism	Test Type	Route	Reported Dose (Normalized Dose)	Effect	Source
rat	LD50	oral	2gm/kg (2000mg/kg)		Scientia Pharmaceutica. Vol. 47, Pg. 39, 1979.

Safety Statements: R36/37/38,

EINECS: 305-879-5

Molecular Formula: C18H9NNa2O8S2

Molecular Weight: 477.38

InChI: InChI=1/C18H11NO8S2.2Na/c20-17-11-3-1-2-4-12(11)18(21)15(17)13-6-5-9-7-10(28(22,23)24)8-14(16(9)19-13)29(25,26)27;;/h1-8,15H,(H,22,23,24)(H,25,26,27);;/q;2*+1/p-2

Risk Statements: S26,S36,

Properties: Yellow to orange-brown powder

Storage Temperature: Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances.

Chemical Properties: Yellow to orange-brown powder

Usage: Textile dye for wool, nylon, silk.

Hazard Symbols  Xi:Irritant

Send FRQ