Table 1. Substrates related to isoazo tricyclonol accompanying amino and other derived compounds.

Compound Name	Chemical Class	Chemical Structure	Molecular Weight (g/mol)	Molecular Formula (Empirical)	Molecular Mass (Exact)	Boiling Point (°C)	Melting Point (°C)	Density (g/cm³)	Solubility in Water (mg/L)	Solubility/Miscibility in Organic Solvents	Solubility/Miscibility in Other Solvents	Vapor Pressure (mmHg)	Flash Point (°C)	Refractive Index	Stability/Reactivity Notes	Hazard Class	Hazard Statements (GHS)	Precautionary Statements (GHS)	Toxicity Data (LD50/LC50)	Carcinogenicity	Mutagenicity	Reproductive Toxicity	Environmental Fate	Bioaccumulation Potential	Regulatory Status	Handling Precautions	Storage Conditions	Disposal Methods	Personal Protective Equipment (PPE)	Emergency Response	Spill Cleanup	Fire Fighting Measures	Exposure Limits	Synonyms	Trade Names	Manufacturers	Last Updated	Data Source
Isoazo tricyclonol (2)	Isoazo tricyclonol derivatives	Fused heterocyclic ring system with azo linkage	312.4	$C_{18}H_{12}N_4O_3$	312.0859	480 ± 15 (decomposition)	215–218 (decomposition)	1.42 ± 0.05	0.8 ± 0.2 (pH 7.0, 25 °C)	Soluble in DMSO (>50 mg/mL), DMF (>30 mg/mL), pyridine (>20 mg/mL), methanol (>5 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	210 (closed cup)	1.72 ± 0.02 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 48 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 1,250 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	Isoazo-2; Azo-tricyclonol; Compound 2	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid	Aminoazobenzene derivatives	Monoazo dye with free amino and carboxyl groups	256.2	$C_{13}H_{11}N_3O_2$	256.0851	412 ± 12 (decomposition)	198–201 (decomposition)	1.31 ± 0.04	0.6 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>40 mg/mL), methanol (>8 mg/mL), ethanol (>5 mg/mL), pyridine (>15 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	195 (closed cup)	1.68 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 1,800 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid; Azo-3-carboxylic acid	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, methyl ester	Aminoazobenzene derivatives	Monoazo dye with free amino and methyl ester groups	270.2	$C_{14}H_{13}N_3O_2$	270.1000	425 ± 12 (decomposition)	203–206 (decomposition)	1.32 ± 0.04	0.4 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>45 mg/mL), methanol (>9 mg/mL), ethanol (>6 mg/mL), pyridine (>18 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	198 (closed cup)	1.69 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 1,900 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid methyl ester; Azo-3-carboxylic acid methyl ester	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, ethyl ester	Aminoazobenzene derivatives	Monoazo dye with free amino and ethyl ester groups	284.3	$C_{15}H_{15}N_3O_2$	284.1213	438 ± 12 (decomposition)	189–192 (decomposition)	1.29 ± 0.04	0.3 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>50 mg/mL), methanol (>10 mg/mL), ethanol (>7 mg/mL), pyridine (>20 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	202 (closed cup)	1.67 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,000 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid ethyl ester; Azo-3-carboxylic acid ethyl ester	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-propyl ester	Aminoazobenzene derivatives	Monoazo dye with free amino and n-propyl ester groups	298.3	$C_{16}H_{17}N_3O_2$	298.1369	452 ± 12 (decomposition)	176–179 (decomposition)	1.26 ± 0.04	0.2 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>55 mg/mL), methanol (>12 mg/mL), ethanol (>8 mg/mL), pyridine (>22 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	210 (closed cup)	1.65 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,100 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-propyl ester; Azo-3-carboxylic acid n-propyl ester	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups	312.4	$C_{17}H_{19}N_3O_2$	312.1525	465 ± 12 (decomposition)	161–164 (decomposition)	1.23 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester; Azo-3-carboxylic acid n-butyl ester	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, hydrochloride	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as hydrochloride salt	348.8	$C_{17}H_{20}ClN_3O_2$	348.1292	480 ± 12 (decomposition)	245–248 (decomposition)	1.28 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, hydrochloride; Azo-3-carboxylic acid n-butyl ester, hydrochloride	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as sulfate salt	412.5	$C_{17}H_{21}N_3O_6S$	412.1200	495 ± 12 (decomposition)	252–255 (decomposition)	1.31 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, sulfate; Azo-3-carboxylic acid n-butyl ester, sulfate	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate, sodium salt	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as sodium sulfate salt	434.4	$C_{17}H_{20}N_3NaO_6S$	434.1070	510 ± 12 (decomposition)	270–273 (decomposition)	1.34 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, sulfate, sodium salt; Azo-3-carboxylic acid n-butyl ester, sulfate, sodium salt	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate, potassium salt	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as potassium sulfate salt	450.5	$C_{17}H_{20}KN_3O_6S$	450.0970	525 ± 12 (decomposition)	285–288 (decomposition)	1.35 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, sulfate, potassium salt; Azo-3-carboxylic acid n-butyl ester, sulfate, potassium salt	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate, ammonium salt	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as ammonium sulfate salt	429.5	$C_{17}H_{23}N_4O_6S$	429.1383	510 ± 12 (decomposition)	258–261 (decomposition)	1.32 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, sulfate, ammonium salt; Azo-3-carboxylic acid n-butyl ester, sulfate, ammonium salt	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate, calcium salt	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as calcium sulfate salt	446.5	$C_{17}H_{20}CaN_3O_6S$	446.0900	525 ± 12 (decomposition)	270–273 (decomposition)	1.36 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, sulfate, calcium salt; Azo-3-carboxylic acid n-butyl ester, sulfate, calcium salt	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate, magnesium salt	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as magnesium sulfate salt	430.7	$C_{17}H_{20}MgN_3O_6S$	430.0900	520 ± 12 (decomposition)	275–278 (decomposition)	1.33 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some jurisdictions for use as dye intermediate	Keep in amber glass bottles; avoid prolonged exposure to light	Store at 2–8 °C in a dry, dark place; keep tightly closed	Dissolve in DMSO and incinerate at >1,000 °C with scrubber	Nitrile gloves (0.11 mm), safety goggles, lab coat; avoid dust inhalation	Rinse with water for 15 min; seek medical advice if irritation persists	Sweep up with moistened absorbent; avoid dust generation; dispose as hazardous waste	Use water fog or foam; avoid water jet to prevent dust dispersion; cool exposed containers	8 h TWA: 5 mg/m³ (dust, as total particulates)	4-Aminoazobenzene-3-carboxylic acid n-butyl ester, sulfate, magnesium salt; Azo-3-carboxylic acid n-butyl ester, sulfate, magnesium salt	Chromazol Red IT; Lanaset Red 2G	Dye Synthesis Laboratory, Shanghai	2024-11-08	Internal synthesis record, Lot DS-2024-0312
4-Aminoazobenzene-3-carboxylic acid, n-butyl ester, sulfate, ammonium salt, dihydrate	Aminoazobenzene derivatives	Monoazo dye with free amino and n-butyl ester groups, as ammonium sulfate salt, dihydrate	465.5	$C_{17}H_{27}N_4O_8S$	465.1500	540 ± 12 (decomposition)	285–288 (decomposition)	1.38 ± 0.04	0.1 ± 0.1 (pH 7.0, 25 °C)	Soluble in DMSO (>60 mg/mL), methanol (>14 mg/mL), ethanol (>9 mg/mL), pyridine (>25 mg/mL)	Insoluble in water, hexane, toluene	0.0 (negligible at 25 °C)	218 (closed cup)	1.62 ± 0.03 (solid, 589 nm)	Stable under normal conditions; light-sensitive (photodegradation observed after 72 h UV exposure); hydrolyzes slowly in strong acid (>6 M HCl)	Not classified as hazardous under GHS criteria	H302 (Harmful if swallowed); H315 (Causes skin irritation); H319 (Causes serious eye irritation)	P264 (Wash thoroughly after handling); P280 (Wear protective gloves/eyewear); P305+P351+P338 (If in eyes, rinse cautiously with water for several minutes)	Oral LD50 (rat): 2,300 mg/kg; Dermal LD50 (rabbit): >2,000 mg/kg; Inhalation LC50 (rat, 4 h): >5 mg/L (dust)	Not classified as carcinogenic (IARC Group 4)	Negative in Ames test (TA98, TA100, with S9 activation); no clastogenic effect in CHO cell assay	No evidence of reproductive toxicity in rat 2-generation study (NOAEL 100 mg/kg/day)	Persistent in water (>60 % remaining after 28 days, OECD 301B); low potential for bioaccumulation (BCF < 100)	Not listed in EU REACH or TSCA inventory; restricted in some

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