SECTION-1: Identification of the substance / mixture and the company / undertaking

Catalogue Number	CS-O-55050
Product Name	1,6-Dinitropyrene
CAS No.	42397-64-8
Category	Nitrosamine
Synonyms	1,6-Dinitropyrene
Brand	Clearsynth Labs Ltd.
Identified uses	Laboratory Chemicals
Uses advised against	Not available
Company	Clearsynth Labs Ltd. Mumbai, India
Emergency Phone #	+91-22-245045900
REACH No.	Not available

SECTION 2: Hazards identification

Disclaimer: This is sample MSDS. Please email **sales@clearsynth.com** for more details.

2.1 Classification of the substance or mixture-Regulation (EC) No 1272/2008:

Not available

2.2 Label Elements

Signal Word: Warning

Hazard Statement(s)

Code	Statement
H350	Not available
H341	Not available
H351	Not available

Precautionary Statement(s)

Code	Statement
P203	Not available
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P318	Not available
P405	Store locked up.
P501	Dispose of contents/container in accordance with local/regional/national/international regulatio

SECTION 3: Composition / information on ingredients

3.1 Substance

Component : 1,6-Dinitropyrene
CAS Number : 42397-64-8
Molecular Formula : C16H8N2O4
Molecular Weight : 292.25
Parent Chemical : Pyrene
Synonyms : 1,6-Dinitropyrene
Concentration : Not available

SECTION 4: First aid measures

Not available

SECTION 5: Firefighting measures

Not available

SECTION 6: Accidental release measures

Not available

SECTION-7: Handling and storage

Not available

SECTION 8: Exposure controls / personal protection

Not available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Test	Result
Appearance	No data available
IR spectrum	No data available
pH	No data available
Solubility	No data available

Property	Value
a) Physical State	No data available
b) Color	No data available
c) Odor	No data available
d) pH	No data available
e) Vapour Pressure	No data available
f) Viscosity	No data available
g) Initial Boiling Point and boiling range	No data available
h) Melting Point / Freezing Point	No data available
i) Auto Ignition Temperature	No data available
j) Flash Point	No data available
k) Explosion Limit, Lower	No data available
l) Explosion Limit, Upper	No data available
m) Decomposition Temperature	No data available
n) Loss on Drying	No data available
o) Relative Density	No data available
p) Solubility (in DMSO)	No data available
q) Oxidizing Properties	No data available

SECTION 10: Stability and reactivity

Not available

SECTION 11: Toxicological information

11.1 Information on toxicological effects
- Acute toxicity: /GENOTOXICITY/ ...The mutagenic ... effects of benzene (B), nitrobenzene (NB), phenol (P), 2-nitrophenol (2-NP), 2,4-dinitrophenol (2,4-DNP), pyrene (Py), 1-nitropyrene (1-NPy), 1,3-dinitropyrene (1,3-DNPy), 1,6-dinitropyrene (1,6-DNPy), and 1,8-dinitropyrene (1,8-DNPy) ... were evaluated with umuC test in presence and in absence of metabolic activation with S9 mix. Then ... both cytokinesis-blocked micronucleus (CBMN) assay, in combination with fluorescent in situ hybridization (FISH) of human pan-centromeric DNA probes on human lymphocytes /were used/ in order to evaluate the genotoxic effects. Analysis of all results shows that nitro polycyclic aromatic hydrocarbons (PAHs) are definitely environmental genotoxic/mutagenic hazards and confirms that environmental aromatic nitration reactions lead to an increase in genotoxicity and mutagenicity properties. Particularly 1-NPy and 1,8-DNPy can be considered as human potential carcinogens... /GENOTOXICITY/ The mutagenicity (trifluorothymidine resistance at the thymidine kinase locus) of 1-, 2-, and 4-nitropyrene (1-, 2-, and 4-NP), 1,3-, 1,6-, and 1,8-dinitropyrene (1,3-, 1,6-, and 1,8-DNP), and pyrene was assessed in a quantitative forward mutation assay using a metabolically competent line (MCL-5) of human B-lymphoblastoid cells. These cells contain endogenous cytochrome P450 activity (CYP1A1) and two plasmids that express cDNAs for four additional P450s (CYP1A2, CYP2A6, CYP2E1, CYP3A4) and microsomal epoxide hydrolase found in human liver. The major finding is that 2-NP and 1,3-DNP, both potent bacterial mutagens, were nonmutagenic in this assay. The following mutagenic potency series, expressed as the minimum detectable mutagen concentration (MDMC) in nmol/mL, was obtained: 1,6-DNP (0.8), 1,8-DNP (1.5), 4-NP (3.1), 1-NP (9.1), 2-NP (> 81), 1,3-DNP (> 86), pyrene (> 494). There was over an 11-fold difference between the most potent (1.6-DNP) and the least potent (1-NP) mutagen. 1,6-DNP was approximately twice as mutagenic as 1,8-DNP, which was almost twice as mutagenic as 4-NP, which, in turn was nearly three times as potent as 1-NP.
- Skin corrosion/irritation: No data available.
- Serious eye damage/eye irritation: No data available.
- Respiratory or skin sensitization: No data available.
- Germ cell mutagenicity: /GENOTOXICITY/ ...The mutagenic ... effects of benzene (B), nitrobenzene (NB), phenol (P), 2-nitrophenol (2-NP), 2,4-dinitrophenol (2,4-DNP), pyrene (Py), 1-nitropyrene (1-NPy), 1,3-dinitropyrene (1,3-DNPy), 1,6-dinitropyrene (1,6-DNPy), and 1,8-dinitropyrene (1,8-DNPy) ... were evaluated with umuC test in presence and in absence of metabolic activation with S9 mix. Then ... both cytokinesis-blocked micronucleus (CBMN) assay, in combination with fluorescent in situ hybridization (FISH) of human pan-centromeric DNA probes on human lymphocytes /were used/ in order to evaluate the genotoxic effects. Analysis of all results shows that nitro polycyclic aromatic hydrocarbons (PAHs) are definitely environmental genotoxic/mutagenic hazards and confirms that environmental aromatic nitration reactions lead to an increase in genotoxicity and mutagenicity properties. Particularly 1-NPy and 1,8-DNPy can be considered as human potential carcinogens... /GENOTOXICITY/ The mutagenicity (trifluorothymidine resistance at the thymidine kinase locus) of 1-, 2-, and 4-nitropyrene (1-, 2-, and 4-NP), 1,3-, 1,6-, and 1,8-dinitropyrene (1,3-, 1,6-, and 1,8-DNP), and pyrene was assessed in a quantitative forward mutation assay using a metabolically competent line (MCL-5) of human B-lymphoblastoid cells. These cells contain endogenous cytochrome P450 activity (CYP1A1) and two plasmids that express cDNAs for four additional P450s (CYP1A2, CYP2A6, CYP2E1, CYP3A4) and microsomal epoxide hydrolase found in human liver. The major finding is that 2-NP and 1,3-DNP, both potent bacterial mutagens, were nonmutagenic in this assay. The following mutagenic potency series, expressed as the minimum detectable mutagen concentration (MDMC) in nmol/mL, was obtained: 1,6-DNP (0.8), 1,8-DNP (1.5), 4-NP (3.1), 1-NP (9.1), 2-NP (> 81), 1,3-DNP (> 86), pyrene (> 494). There was over an 11-fold difference between the most potent (1.6-DNP) and the least potent (1-NP) mutagen. 1,6-DNP was approximately twice as mutagenic as 1,8-DNP, which was almost twice as mutagenic as 4-NP, which, in turn was nearly three times as potent as 1-NP.
- Carcinogenicity: There is sufficient evidence for the carcinogenicity in experimental animals of 1,6-dinitropyrene. No data were available from studies in humans on the carcinogenicity of 1,6-dinitropyrene. Overall evaluation:

1,6-Dinitropyrene is possibly carcinogenic to humans (Group 2B). 1,6-Dinitropyrene is reasonably anticipated to be a human carcinogen based on sufficient evidence of malignant tumor formation in multiple species of experimental animals, at multiple sites and by multiple routes of exposure.
- Reproductive toxicity: No data available.
- STOT-single exposure: No data available.
- STOT-repeated exposure: /LABORATORY ANIMALS: Chronic Exposure or Carcinogenicity/ Eight nitropolycyclic aromatic hydrocarbons (PAHs), including ... 1,6- and 1,8-dinitropyrene, ... were tested for tumorigenicity in the newborn mouse model by ip administration at 1, 8, and 15 days after birth. ... Female mice treated with 200 nmol of ... 1,6- or 1,8-dinitropyrene did not develop liver tumors but the hepatic tumor incidence in males was ... 32 and 16%, respectively... /LABORATORY ANIMALS: Chronic Exposure or Carcinogenicity/ The carcinogenicities of 1-nitropyrene (1-NP), 4-nitropyrene (4-NP), 1,3-dinitropyrene (1,3-DNP), 1,6-dinitropyrene (1,6-DNP), 1,8-dinitropyrene (1,8-DNP), 3-hydroxy-1-nitropyrene (3-OH-1-NP) and a mixture of 6- and 8-hydroxy-1-nitropyrene (6/8-OH-1-NP) were investigated in ... newborn female CD rats treated sc eight times at weekly intervals with a total dose of 6.3 umol ... control animals received only dimethylsulfoxide (DMSO). The experiment was terminated at 67 weeks. With the exception of 1,6-DNP- and 1,8-DNP-treated animals, which had average survival periods of 149 and 164 days respectively, the animals administered the other compounds did not show decreased survival. Malignant fibrous histiocytomas were observed in 12%, 100% and 100% of the rats treated with 1,3-, 1,6- and 1,8-DNP respectively. Leukemia was found in 20% and 22% of the animals treated with 1,6- and 1,8-DNP respectively. No control rats developed these tumors. Additionally, mammary tumors were induced in rats treated with 1-NP. Newborn female CD rats were similarly treated with 1-NP, 4-NP, 3-OH-1-NP, 6/8-OH-1-NP or DMSO and newborn female F344 rats were treated with 1-NP or DMSO. The experiment was terminated at 86 weeks, 1-NP and 4-NP produced mammary adenocarcinoma in CD rats. Although 1-NP did not produce mammary adenocarcinoma in F344 rats, it induced leukemia. 4-NP also induced malignant fibrous histiocytomas in CD rats. This study demonstrates that 4-NP is more carcinogenic than 1-NP and that CD rats are more susceptible than F344 rats to mammary carcinogenesis by 1-NP. Additionally, 1,6- and 1,8-DNP are more potent than 1-NP in inducing malignant fibrous histiocytomas and leukemia.
- Aspiration hazard: No data available.

Likely routes of exposure
- 1,6-Dinitropyrene is reasonably anticipated to be a human carcinogen based on sufficient evidence of malignant tumor formation in multiple species of experimental animals, at multiple sites and by multiple routes of exposure.

Symptoms related to the physical, chemical and toxicological characteristics
- /GENOTOXICITY/ ...The mutagenic ... effects of benzene (B), nitrobenzene (NB), phenol (P), 2-nitrophenol (2-NP), 2,4-dinitrophenol (2,4-DNP), pyrene (Py), 1-nitropyrene (1-NPy), 1,3-dinitropyrene (1,3-DNPy), 1,6-dinitropyrene (1,6-DNPy), and 1,8-dinitropyrene (1,8-DNPy) ... were evaluated with umuC test in presence and in absence of metabolic activation with S9 mix. Then ... both cytokinesis-blocked micronucleus (CBMN) assay, in combination with fluorescent in situ hybridization (FISH) of human pan-centromeric DNA probes on human lymphocytes /were used/ in order to evaluate the genotoxic effects. Analysis of all results shows that nitro polycyclic aromatic hydrocarbons (PAHs) are definitely environmental genotoxic/mutagenic hazards and confirms that environmental aromatic nitration reactions lead to an increase in genotoxicity and mutagenicity properties. Particularly 1-NPy and 1,8-DNPy can be considered as human potential carcinogens...

SECTION 12: Ecological information

Not available

SECTION 13: Disposal considerations

Not available

SECTION 14: Transport information

Not available

SECTION 15: Regulatory information

Not available

SECTION 16: Other information

Not available

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