Phenol, 4,4'-(1,2-diethyl-1,2-ethanediyl)bis-, rel- (cas 84-16-2) MSDS

**MSDS**

**CAS:** 84-16-2

**SYNONYMS:**
- Bibenzyl, alpha, alpha'-diethyl-4,4'-dihydroxy-
- meso-3,4-Bis(p-hydroxyphenyl)-n-hexane
- 3,4-Bis(p-hydroxyphenyl)hexane
- Cycloestrol
- 4,4'-(1,2-Diethylethylene)diphenol
- Phenol, 4,4'-(1,2-diethyl-1,2-ethanediyl)bis-, (R*,S*)-
- Dihydrodiethylstilbestrol
- Dihydrostilbestrol
- 4,4'-Dihydroxy-alpha,beta-diethylidiphenylethane
- 4,4'-Dihydroxy-gamma,delta-diphenylhexane
- gamma,delta-Di(p-hydroxyphenyl)-hexane
- meso-3,4-Di(p-hydroxyphenyl)-n-hexane
- Extra-plex
- Hexane, 3,4-bis(p-hydroxyphenyl)-
- Hexanoestrol
- Hexestrol
- meso-Hexestrol
- Hexoestrol
- Hormoestrol
- Sinestrol
- Stilbestrol, dihydro-
- Synestrol
- Synthovo
- Syntrogene
- Vitestrol
MOLECULAR FORMULA: C18-H22-O2
MOLECULAR WEIGHT: 270.40
WISWESSER LINE NOTATION: QR DY2&Y2&R DQ
COMPOUND DESCRIPTOR: Tumorigen
Drug
Mutagen
Reproductive Effector
Hormone
SYNONYMS/TRADE NAMES:
* Bibenzyl, alpha,alpha'-diethyl-4,4'-dihydroxy-
* meso-3,4-Bis(p-hydroxyphenyl)-n-hexane
* 3,4-Bis(p-hydroxyphenyl)hexane
* Cycloestrol
* 4,4'-(1,2-Diethylethylene)diphenol
* Phenol, 4,4'-(1,2-diethyl-1,2-ethylenediyl)bis-, (R*,S*)-
* Dihydrodiethylstilbestrol
* Dihydrostilbestrol
* 4,4'-Dihydroxy-alpha,beta-diethyldiphenylethene
* 4,4'-Dihydroxy-gamma,delta-diphenylhexane
* gamma,delta-Di(p-hydroxyphenyl)-hexane
* meso-3,4-Di(p-hydroxyphenyl)-n-hexane
* Extra-plex
* Hexane, 3,4-bis{p-hydroxyphenyl}-
* Hexanoestrol
* Hexestrol
* meso-Hexestrol
* Hexoestrol
* Hormoestrol
* Sinestrol
* Stilbestrol, dihydro-
* Synestrol
* Synthovo
* Syntro gene
* Vitestrol

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST: LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE: Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : >2 gm/kg

TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value

REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,744,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 200 mg/kg

TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value

REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,743,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 1 gm/kg

TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value

REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,743,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 1 gm/kg

TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value

REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,743,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 200 mg/kg

TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
TYPE OF TEST: LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE: Subcutaneous
SPECIES OBSERVED: Rodent - mouse
DOSE/DURATION: >3 gm/kg

TOXIC EFFECTS:
Details of toxic effects not reported other than lethal dose value

** OTHER MULTIPLE DOSE TOXICITY DATA **

TYPE OF TEST: TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE: Oral
SPECIES OBSERVED: Rodent - rat
DOSE/DURATION: 19500 mg/kg/26W-I

TOXIC EFFECTS:
Endocrine - changes in pituitary weight
Nutritional and Gross Metabolic - weight loss or decreased weight gain
Related to Chronic Data - changes in uterine weight

REFERENCES:
NIIDRN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,743,1982

NIIDRN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,744,1982


DOSE/DURATION : 2520 mg/kg/42D-I

TOXIC EFFECTS:
- liver - changes in liver weight
- Endocrine - changes in pituitary weight
- Related to Chronic Data - changes in uterine weight

REFERENCE:

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 270 mg/kg/27D-I

TOXIC EFFECTS:
- Kidney, Ureter, Bladder - other changes in urine composition
- Blood - normocytic anemia
- Biochemical - Metabolism (Intermediary) - lipids including transport

REFERENCE:

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 540 mg/kg/90D-I

TOXIC EFFECTS:
- Behavioral - food intake (animal)
- Blood - normocytic anemia
- Nutritional and Gross Metabolic - weight loss or decreased weight gain

REFERENCE:

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 540 mg/kg/90D-I

TOXIC EFFECTS:
- Kidney, Ureter, Bladder - other changes in urine composition
- Blood - normocytic anemia
- Nutritional and Gross Metabolic - weight loss or decreased weight gain
** TUMORIGENIC DATA **

** TYPE OF TEST **
- TDLo - Lowest published toxic dose

** ROUTE OF EXPOSURE **
- Subcutaneous

** SPECIES OBSERVED **
- Rodent - mouse

** DOSE/DURATION **
- 74 mg/kg/56W-I

** TOXIC EFFECTS :**
- Tumorigenic - Carcinogenic by RTECS criteria
- Skin and Appendages - tumors

** REFERENCE :**
YACHDS Yakuri to Chiryo. Pharmacology and Therapeutics. (Raifu Saiensu Shuppan K.K, 2-5-13, Yaesu, Chuo-ku, Tokyo 104, Japan) V.1- 1972-
Volume(issue)/page/year: 7,3355,1979

---

** TYPE OF TEST **
- TDLo - Lowest published toxic dose

** ROUTE OF EXPOSURE **
- Intravaginal

** SPECIES OBSERVED **
- Rodent - mouse

** DOSE/DURATION **
- 18 mg/kg/17W-I

** TOXIC EFFECTS :**
- Tumorigenic - neoplastic by RTECS criteria
- Reproductive - Tumorigenic effects - ovarian tumors

** REFERENCE :**

---

** TYPE OF TEST **
- TDLo - Lowest published toxic dose

** ROUTE OF EXPOSURE **
- Subcutaneous

** SPECIES OBSERVED **
- Rodent - guinea pig

** DOSE/DURATION **
- 74 mg/kg/69W-I

** TOXIC EFFECTS :**
- Tumorigenic - neoplastic by RTECS criteria
- Skin and Appendages - tumors

** REFERENCE :**
VOONAW Voprosy Onkologii. Problems of Oncology. For English translation, see PONCAU. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) V.1-10, 1928-37; V.1- 1955- Volume(issue)/page/year: 22(3),68,1976

---

** TYPE OF TEST **
- TDLo - Lowest published toxic dose

** ROUTE OF EXPOSURE **
- Implant

** REFERENCES :**
SPECIES OBSERVED        : Rodent - guinea pig
DOSE/DURATION           : 540 ug/kg

TOXIC EFFECTS :
  Tumorigenic - equivocal tumorigenic agent by RTECS criteria
  Reproductive - Tumorigenic effects - uterine tumors

REFERENCE :
  BSBSAS Boletin de la Sociedad de Biologia de Santiago de Chile. (Santiago, Chile) V.1-12, 1943-55. Discontinued. Volume(issue)/page/year: 8,142,1951

TYPE OF TEST            : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE       : Subcutaneous
SPECIES OBSERVED        : Rodent - hamster
DOSE/DURATION           : 360 mg/kg

TOXIC EFFECTS :
  Tumorigenic - equivocal tumorigenic agent by RTECS criteria
  Kidney, Ureter, Bladder - Kidney tumors

REFERENCE :

TYPE OF TEST            : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE       : Implant
SPECIES OBSERVED        : Rodent - hamster
DOSE/DURATION           : 640 mg/kg/38W-I

TOXIC EFFECTS :
  Tumorigenic - equivocal tumorigenic agent by RTECS criteria
  Kidney, Ureter, Bladder - Kidney tumors

REFERENCE :

TYPE OF TEST            : TD - Toxic dose (other than lowest)
ROUTE OF EXPOSURE       : Subcutaneous
SPECIES OBSERVED        : Rodent - hamster
DOSE/DURATION           : 800 mg/kg/26W-I

TOXIC EFFECTS :
  Tumorigenic - equivocal tumorigenic agent by RTECS criteria
  Kidney, Ureter, Bladder - Kidney tumors

REFERENCE :
  VOONAW Voprosy Onkologii. Problems of Oncology. For English translation, see PONCAU. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) V.1-10, 1928-37; V.1-    1955- Volume(issue)/page/year: 7(7),35,1961
** REPRODUCTIVE DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE : 250 ug/kg
SEX/DURATION : female 5 day(s) pre-mating

TOXIC EFFECTS :
Reproductive - Fertility - female fertility index (e.g. # females pregnant per # sperm positive females; # females pregnant per # females mated)

REFERENCE :
CHTPBA Chimica Therapeutica. (Paris, France) V.1-8, 1965-73. For publisher information, see EJMCA5. Volume(issue)/page/year: 4,1,1969

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE : 3 mg/kg
SEX/DURATION : female 19-21 day(s) after conception

TOXIC EFFECTS :
Reproductive - Specific Developmental Abnormalities - urogenital system
Reproductive - Effects on Newborn - stillbirth

REFERENCE :

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE : 546 mg/kg
SEX/DURATION : female 91 day(s) pre-mating

TOXIC EFFECTS :
Reproductive - Maternal Effects - ovaries, fallopian tubes
Reproductive - Maternal Effects - uterus, cervix, vagina

REFERENCE :

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Unreported
SPECIES OBSERVED : Rodent - guinea pig
DOSE : 150 mg/kg
SEX/DURATION : female 21 week(s) pre-mating
TOXIC EFFECTS :
Reproductive - Maternal Effects - uterus, cervix, vagina
REFERENCE :
BEXBAN Bulletin of Experimental Biology and Medicine (English Translation).
Translation of BERMAZ. (Plenum Pub. Corp., 233 Spring St., New York, NY
10013) V.41- 1956- Volume(issue)/page/year: 94,1713,1982

** MUTATION DATA **

TYPE OF TEST : Unscheduled DNA synthesis
ROUTE OF EXPOSURE : Subcutaneous
TEST SYSTEM : Rodent - mouse
DOSE/DURATION : 400 mg/kg
REFERENCE :
CNREA8 Cancer Research. (Public Ledger Building, Suit 816, 6th & Chestnut

TYPE OF TEST : DNA damage
TEST SYSTEM : Rodent - hamster Embryo
DOSE/DURATION : 3 mg/L
REFERENCE :
CRNGDP Carcinogenesis (London). (Oxford Univ. Press, Pinkhill House,
Southfield Road, Eynsham, Oxford OX8 1JJ, UK) V.1- 1980-
Volume(issue)/page/year: 7,1329,1986

TYPE OF TEST : Unscheduled DNA synthesis
TEST SYSTEM : Rodent - hamster Embryo
DOSE/DURATION : 1 mg/L
REFERENCE :
CNREA8 Cancer Research. (Public Ledger Building, Suit 816, 6th & Chestnut
Sts., Philadelphia, PA 19106) V.1- 1941- Volume(issue)/page/year:
44,184,1984

TYPE OF TEST : Sex chromosome loss and nondisjunction
TEST SYSTEM : Rodent - hamster Fibroblast
DOSE/DURATION : 75 umol/L
REFERENCE :
MUREAV Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE
Amsterdam, Netherlands) V.1- 1964- Volume(issue)/page/year: 171,31,1986
*** REVIEWS ***

IARC Cancer Review: Animal Sufficient Evidence
IMSUDL IARC Monographs, Supplement. (WHO Publications Centre USA, 49 Sheridan Ave., Albany, NY 12210) No.1- 1979- Volume(issue)/page/year:
7,279,1987

*** END OF RECORD ***