



chemists helping chemists in research & industry

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P O BOX 296
WHITEWATER WI 53190

DATE: 01/12/90
CUST#: 523216
PO#: UNJ-02446

MATERIAL SAFETY DATA SHEET

PAGE 1

IDENTIFICATION

PRODUCT #: C5-3 NAME: CAFFEINE, 99%
CAS #: 58-08-2
MF: C8H10N4O2

SYNONYMS

CAFFEIN * COFFEIN (GERMAN) * COFFEINE * 3,7-DIHYDRO-1,3,7-TRIMETHYL-
1H-PURINE-2,6-DIONE * ELDIATRIC C * GUARANINE * KOFEIN (CZECH) *
KOFFEIN (GERMAN) * METHYLTHEOBROMIDE * NCI-C02733 * NO-DOZ * ORGANEX *
1H-PURINE-2,6-DIONE, 3,7-DIHYDRO-1,3,7-TRIMETHYL- * THEIN * THEINE *
THEOBROMINE, 1-METHYL- * THEOPHYLLINE, 7-METHYL * 1,3,7-TRIMETHYL-2,6-
DIOXOPURINE * 1,3,7-TRIMETHYLXANTHINE * XANTHINE, 1,3,7-TRIMETHYL *

TOXICITY HAZARDS

RTECS NO: EV6475000

CAFFEINE

TOXICITY DATA

ORL-HMN LD01:192 MG/KG
ORL-CHD LD01:320 MG/KG
ORL-WMN LD01:1 GM/KG
IVN-WMN LD01:57 MG/KG
ORL-RAT LD50:192 MG/KG
IPR-RAT LD50:260 MG/KG
SCU-RAT LD50:170 MG/KG
IVN-RAT LD50:105 MG/KG
REC-RAT LD50:300 MG/KG
ORL-MUS LD50:127 MG/KG
IPR-MUS LD50:168 MG/KG
SCU-MUS LD50:242 MG/KG
IVN-MUS LD50:62 MG/KG
UNR-MUS LD50:251 MG/KG
ORL-DOG LD50:140 MG/KG
SCU-DOG LD50:100 MG/KG
ORL-RBT LD50:224 MG/KG
IVN-RBT LD50:58 MG/KG
ORL-GPG LD50:230 MG/KG
ORL-HAM LD50:230 MG/KG
ORL-BWD LD50:316 MG/KG

JNDRAK 5,252,65
FNCA6 3,275,74
BIATDR -6,73
APTOA6 15,331,59
JNDRAK 5,252,65
ZERNAL 15,64,76
JCPH88 7,131,67
JPETAB 82,89,44
JCPH88 7,131,67
TXAPA9 44,1,78
CPBTAL 22,1459,74
ARZNAO 6,601,56
TOLED5 29,25,85
NYKZAU 53,25,57
NIIRON 6,174,82
NIIRON 6,174,82
TXAPA9 44,1,78
KSRNAM 13,791,79
TXAPA9 2,23,60
TXAPA9 44,1,78
AECTCV 12,355,83

REVIEWS, STANDARDS, AND REGULATIONS

EPA GENETOX PROGRAM 1988, POSITIVE: CELL TRANSFORM.-SA7/SHE; IN VITRO
CYTOGENETICS-NONHUMAN
EPA GENETOX PROGRAM 1988, POSITIVE: D MELANOGASTER-WHOLE SEX CHROM.
LOSS
EPA GENETOX PROGRAM 1988, POSITIVE: D MELANOGASTER-NONDISJUNCTION; N
CRASSA-ANEUPLOIDY
EPA GENETOX PROGRAM 1988, POSITIVE: E COLI POLA WITHOUT S9; IN VITRO
SCE-HUMAN
EPA GENETOX PROGRAM 1988, POSITIVE: D MELANOGASTER SEX-LINKED LETHAL;
S CEREVISIAE-ANEUPLOIDY
EPA GENETOX PROGRAM 1988, POSITIVE/DOSE RESPONSE: IN VITRO
CYTOGENETICS-HUMAN LYMPHOCYTE

CONTINUED ON NEXT PAGE

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M A T E R I A L S A F E T Y D A T A S H E E T

PAGE 2

CUST#: 523216
PO#: UNJ-02446

PRODUCT #: C5-3
CAS #: 58-08-2
MF: CBH10N402

NAME: CAFFEINE, 99%

TOXICITY HAZARDS

EPA GENETOX PROGRAM 1988, NEGATIVE: SHE-CLONAL ASSAY; RODENT DOMINANT LETHAL
 EPA GENETOX PROGRAM 1988, NEGATIVE: HISTIDINE REVERSION-AMES TEST; IN VITRO SCE-NONHUMAN
 EPA GENETOX PROGRAM 1988, NEGATIVE: MOUSE SPECIFIC LOCUS; SPERM MORPHOLOGY-MOUSE
 EPA GENETOX PROGRAM 1988, NEGATIVE: UDS IN MOUSE GERM CELLS; V79 CELL CULTURE-GENE MUTATION
 EPA GENETOX PROGRAM 1988, NEGATIVE: TRP REVERSION
 EPA GENETOX PROGRAM 1988, NEGATIVE/LIMITED: CARCINOGENICITY-MOUSE/RAT
 EPA GENETOX PROGRAM 1988, INCONCLUSIVE: IN VIVO CYTOGENETICS-NONHUMAN BONE MARROW
 EPA GENETOX PROGRAM 1988, INCONCLUSIVE: CYTOGENETICS-MALE GERM CELL
 EPA GENETOX PROGRAM 1988, INCONCLUSIVE: RODENT HERITABLE TRANSLOCATION; MAMMALIAN MICRONUCLEUS
 EPA GENETOX PROGRAM 1988, INCONCLUSIVE: MOUSE SPOT TEST; B SUBTILIS REC ASSAY
 EPA GENETOX PROGRAM 1988, INCONCLUSIVE: IN VITRO SCE-HUMAN LYMPHOCYTES; IN VIVO SCE-NONHUMAN
 EPA TSCA CHEMICAL INVENTORY, 1986
 EPA TSCA TEST SUBMISSION (TSCATS) DATA BASE, SEPTEMBER 1989

TARGET ORGAN DATA

BEHAVIORAL (SOMNOLENCE)
 BEHAVIORAL (HALLUCINATIONS, DISTORTED PERCEPTIONS)
 BEHAVIORAL (TOXIC PSYCHOSIS)
 BEHAVIORAL (TREMOR)
 BEHAVIORAL (CONVULSIONS OR EFFECT ON SEIZURE THRESHOLD)
 BEHAVIORAL (CHANGE IN MOTOR ACTIVITY)
 BEHAVIORAL (ATAXIA)
 BEHAVIORAL (MUSCLE CONTRACTION OR SPASTICITY)
 BEHAVIORAL (AGGRESSION)
 VASCULAR (BP ELEVATION NOT CHARACTERIZED IN AUTONOMIC SECTION)
 LUNGS, THORAX OR RESPIRATION (DYSPNAE)
 LUNGS, THORAX OR RESPIRATION (RESPIRATORY DEPRESSION)
 GASTROINTESTINAL (HYPERMOTILITY, DIARRHEA)
 GASTROINTESTINAL (NAUSEA OR VOMITING)
 KIDNEY, URETER, BLADDER (URINE VOLUME INCREASED)
 EFFECTS ON FERTILITY (FEMALE FERTILITY INDEX)
 EFFECTS ON FERTILITY (POST-IMPLANTATION MORTALITY)
 EFFECTS ON FERTILITY (LITTER SIZE)
 EFFECTS ON FERTILITY (ABORTION)
 EFFECTS ON EMBRYO OR FETUS (EXTRA EMBRYONIC STRUCTURES)
 EFFECTS ON EMBRYO OR FETUS (MATERNAL-FETAL EXCHANGE)
 EFFECTS ON EMBRYO OR FETUS (FETOTOXICITY)
 EFFECTS ON EMBRYO OR FETUS (FETAL DEATH)
 SPECIFIC DEVELOPMENTAL ABNORMALITIES (CENTRAL NERVOUS SYSTEM)
 SPECIFIC DEVELOPMENTAL ABNORMALITIES (EYE, EAR)

CONTINUED ON NEXT PAGE

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M A T E R I A L S A F E T Y D A T A S H E E T

PAGE 3

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PO#: UNJ-02446

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CAS #: 58-08-2
MF: C8H10N4O2

NAME: CAFFEINE, 99%

TOXICITY HAZARDS

SPECIFIC DEVELOPMENTAL ABNORMALITIES (CRANIOFACIAL)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (SKIN AND SKIN APPENDAGES)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (MUSCULOSKELETAL SYSTEM)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (BLOOD AND LYMPHATIC SYSTEMS)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (GASTROINTESTINAL SYSTEM)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (UROGENITAL SYSTEM)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (HOMEDSTASIS)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (OTHER DEVELOPMENTAL
ABNORMALITIES)
EFFECTS ON NEWBORN (VIABILITY INDEX)
EFFECTS ON NEWBORN (WEANING OR LACTATION INDEX)
EFFECTS ON NEWBORN (GROWTH STATISTICS)
EFFECTS ON NEWBORN (BIOCHEMICAL AND METABOLIC)
EFFECTS ON NEWBORN (BEHAVIORAL)
EFFECTS ON NEWBORN (PHYSICAL)
EFFECTS ON NEWBORN (OTHER POSTNATAL MEASURES OR EFFECTS)

ONLY SELECTED REGISTRY OF TOXIC EFFECTS OF CHEMICAL SUBSTANCES (RTECS)
DATA IS PRESENTED HERE. SEE ACTUAL ENTRY IN RTECS FOR COMPLETE INFORMATION.

HEALTH HAZARD DATA

ACUTE EFFECTS

HARMFUL IF SWALLOWED, INHALED, OR ABSORBED THROUGH SKIN.
MAY CAUSE IRRITATION.

CHRONIC EFFECTS

OVEREXPOSURE MAY CAUSE REPRDOUCTIVE DISORDER(S) BASED ON TESTS WITH
LABORATORY ANIMALS.
LABORATORY EXPERIMENTS HAVE SHOWN MUTAGENIC EFFECTS.

TARGET ORGAN(S):

CENTRAL NERVOUS SYSTEM

HEART

FIRST AID

IN CASE OF CONTACT, IMMEDIATELY FLUSH EYES OR SKIN WITH COPIOUS
AMOUNTS OF WATER FOR AT LEAST 15 MINUTES WHILE REMOVING CONTAMINATED
CLOTHING AND SHOES.

IF INHALED, REMOVE TO FRESH AIR. IF NOT BREATHING GIVE ARTIFICIAL
RESPIRATION. IF BREATHING IS DIFFICULT, GIVE OXYGEN.

CALL A PHYSICIAN.

WASH CONTAMINATED CLOTHING BEFORE REUSE.

PHYSICAL DATA

MELTING PT: 234 C TO 236.5 C

APPEARANCE AND ODOR
WHITE POWDER

FIRE AND EXPLOSION HAZARD DATA

EXTINGUISHING MEDIA
CARBON DIOXIDE.

CONTINUED ON NEXT PAGE

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----- FIRE AND EXPLOSION HAZARD DATA -----

DRY CHEMICAL POWDER.
WATER SPRAY.

SPECIAL FIREFIGHTING PROCEDURES
WEAR SELF-CONTAINED BREATHING APPARATUS AND PROTECTIVE CLOTHING TO
PREVENT CONTACT WITH SKIN AND EYES.

UNUSUAL FIRE AND EXPLOSIONS HAZARDS
EMITS TOXIC FUMES UNDER FIRE CONDITIONS.

----- REACTIVITY DATA -----

INCOMPATIBILITIES
STRONG OXIDIZING AGENTS
HAZARDOUS COMBUSTION OR DECOMPOSITION PRODUCTS
THERMAL DECOMPOSITION MAY PRODUCE CARBON MONOXIDE, CARBON DIOXIDE,
AND NITROGEN OXIDES.

----- SPILL OR LEAK PROCEDURES -----

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED
WEAR RESPIRATOR, CHEMICAL SAFETY GOGGLES, RUBBER BOOTS AND HEAVY
RUBBER GLOVES.
SWEEP UP, PLACE IN A BAG AND HOLD FOR WASTE DISPOSAL.
AVOID RAISING DUST.
VENTILATE AREA AND WASH SPILL SITE AFTER MATERIAL PICKUP IS COMPLETE.

WASTE DISPOSAL METHOD
DISSOLVE OR MIX THE MATERIAL WITH A COMBUSTIBLE SOLVENT AND BURN IN A
CHEMICAL INCINERATOR EQUIPPED WITH AN AFTERBURNER AND SCRUBBER.
OBSERVE ALL FEDERAL, STATE, AND LOCAL LAWS.

--- PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE ---

WEAR APPROPRIATE NIOSH/MSHA-APPROVED RESPIRATOR, CHEMICAL-RESISTANT
GLOVES, SAFETY GOGGLES, OTHER PROTECTIVE CLOTHING.
USE ONLY IN A CHEMICAL FUME HOOD.
SAFETY SHOWER AND EYE BATH.
DO NOT BREATHE DUST.
AVOID CONTACT WITH EYES, SKIN AND CLOTHING.
AVOID PROLONGED OR REPEATED EXPOSURE.
WASH THOROUGHLY AFTER HANDLING.
TOXIC.
POSSIBLE TERATOGEN.
POSSIBLE MUTAGEN.
KEEP TIGHTLY CLOSED.
STORE IN A COOL DRY PLACE.

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M A T E R I A L S A F E T Y D A T A S H E E T

PAGE 5

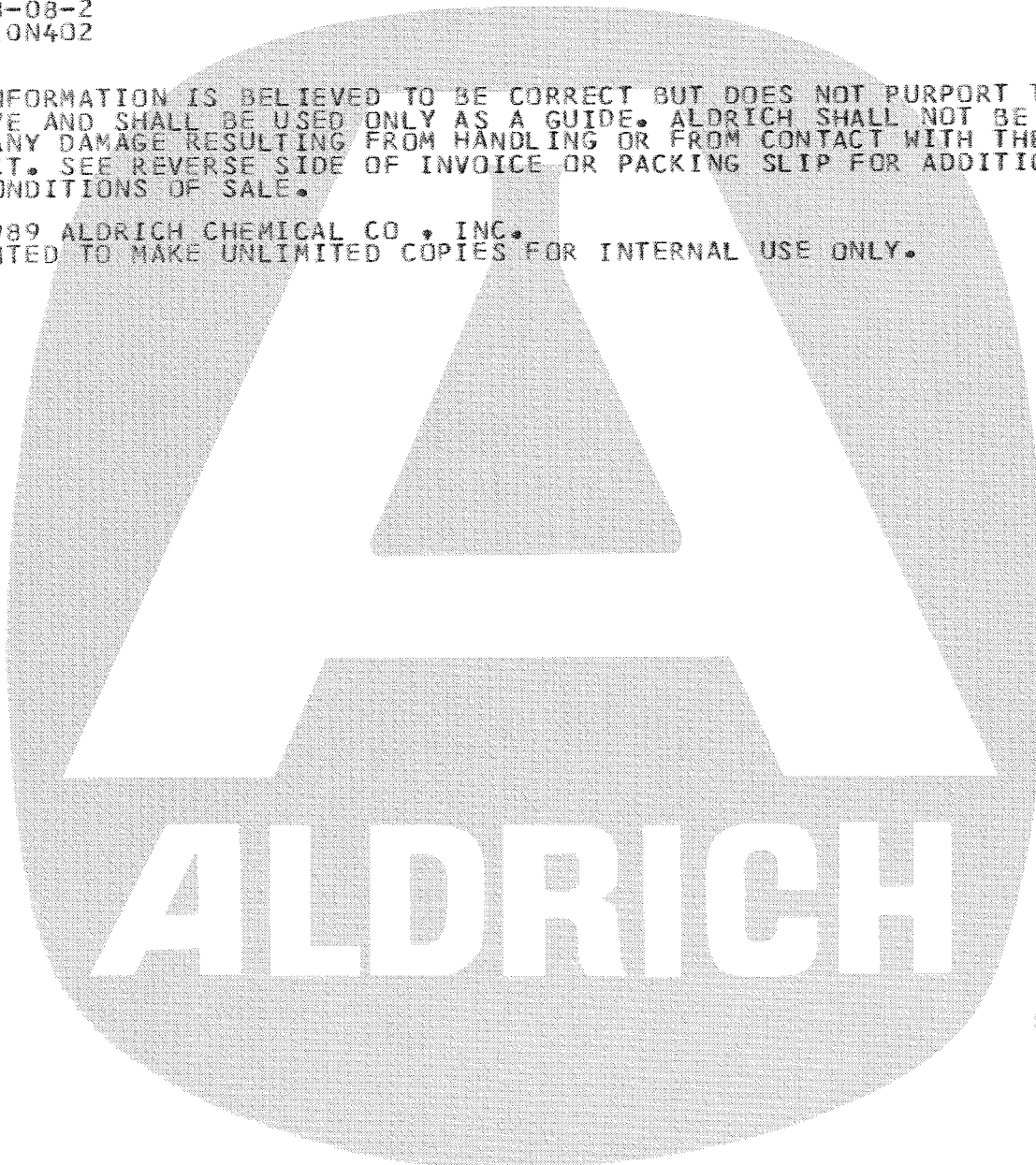
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