

Dictionary of Substances and Their Effects (DOSE)

FILE DESCRIPTION

The **Dictionary of Substances and their Effects (DOSE)** is a unique guide to the impact of chemicals on organisms and the environment. DOSE contains detailed records for more than 4000 chemicals. These chemicals have been selected from sources such as Europe's Black List and Grey List of dangerous substances, the UK's Red List, priority pollutant lists from the USA and Canada, and the pollutant list from Germany. Other chemicals which are reported to have adverse effects on the environment are also covered.

SUBJECT COVERAGE

DOSE includes the following data and information:

- CAS® Registry Number
- Chemical Name and Synonyms
- Chemical Name and Synonyms
- Environmental Fate: Abiotic Removal; Absorption; Anaerobic Effects; Carbonaceous Inhibition; Degradation Studies; Nitrification Inhibition
- Physical and Chemical Properties
- Reference List
- Regulatory Information: Conveyance Classification; EINECS/ELINCS Numbers; HAZCHEM Code; Occupational Exposure; Limit Values; Risk and Safety Phrases; RTECS Numbers; Supply Classification; UN Number
- Toxicity: Ecotoxicity which includes Fish Toxicity; Invertebrate Toxicity; Bioaccumulation Data; Mammalian and Avian Toxicity which includes Carcinogenicity and Long-term Effects; Genotoxicity; Irritancy; Metabolism and Pharmacokinetics; Sensitisation; Teratogenicity and Reproductive Effects; Other Adverse Effects
- Uses

TIPS

USE FILE 307

to identify the hazards of chemicals to both mammals and the environment and to make rapid hazard assessment on a chemical which leads to risk assessment and beyond.

USE MAP

to expand a search to other databases. Use SY (Synonyms), RN (CAS® Registry Number), or SYRN (combination of both) as the field(s) to be extracted from records into a SearchSave, which is then executed in other files.

MAP SYRN TEMP
BEGIN TOXICOL; EXS

USE /NA, NA=

to isolate a particular chemical or substance by name.

EXPAND
NA=1,8-ETHYLENENAPHTHALENE

USE RN=

to retrieve substances by CAS® Registry Number.

DIALOG FILE DATA

Inclusive Dates: Current
Update Frequency: Closed
File Size: 4,123 records as of March 2001

CONTACT

The Dictionary of Substances and their Effects (DOSE) database is provided by the Royal Society of Chemistry. Questions concerning file content should be directed to:

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File 307 Dictionary of Substances and Their Effects (DOSE)
SAMPLE RECORD

DIALOG(R)File 307:DOSE
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AA= 00000810 Record Id: 1359
/CN,CN=,/NA,NA= SUBSTANCE NAME: styrene oxide
RN= CAS REGISTRY NUMBER 96-09-3
/NA,NA=,/SY,SY= SYNONYMS: phenyloxirane; (epoxyethyl)benzene; 1,2-epoxy-
1-phenylethane; epoxystyrene; phenethylene oxide; styryl
oxide; phenyl oxirane
US=,/US USES: In manufacture of styrene glycol and derivatives. In
manufacture of epoxy resins, beta-phenethyl alcohol,
polyols and agrochemicals. In treatment of textiles and
fibres.
/OC,OC= OCCURS: Tentatively identified in US air samples (1,2). In effluent from
latex and chemical plants (3).
/PP PHYSICAL PROPERTIES:
MW= MOLECULAR WEIGHT: 120.15
MF=,EC=,/EC, MOLECULAR FORMULA: C8H8O
ME=,NC=,NE= MELTING POINT: -35.6 Deg C
MP=,MT= BOILING POINT: 194 Deg C
BP=,BT= VAPOR PRESSURE: v.p. 0.3 mmHg at 20 Deg C ; v.den. 4.1
VP=,VT= DENSITY: d(16)4 1.0523
DN=,DT= PARTITION COEFFICIENT: log Pow 1.61
PI=,PT= SOLUBILITY WATER (NUMERIC): 0.3%
SL= SOLUBILITY OTHER SOLVENTS: ethanol, diethyl ether,
benzene, acetone, carbon tetrachloride, heptane,
methanol
FP=,FT= FLASH POINT: 79 Deg C (open cup)
/RG REGULATORY:
REGULATORY NUMBERS:
NI=,RR= NIOSH Number: CZ 9625000
EI= EINECS/ELINCS No.: 202-476-7
Supply Classification: toxic
Risk Phrases: May cause cancer -Harmful in contact
with skin -Irritating to the eyes (R45, R21, R36)
Safety Phrases: Restricted to professional users
-Avoid exposure -obtain special instruction before
use -In case of accident or if you feel unwell, seek
medical advice immediately (show label where possible)
(S53, S45)
/TO TOXICITY:
MAMMALIAN AND AVIAN TOXICITY:
ACUTE TOXICITY: LD50 oral mouse, rat 1500, 2000 mg
kg(-1), respectively (5,6). LCLo (4 hr) inhalation
rat 500 ppm (7). LD50 dermal rabbit 1060 mg kg(-1)
(7). LD50 intraperitoneal rat 460 mg kg(-1) (8).
SUB-CHRONIC TOXICITY: Mortality was high in rats
inhaling 97 or 300 ppm 7 hr day(-1) for 3 wk
pregestational period and on gestation days 1-19
(9,10).
CARCINOGENICITY AND CHRONIC EFFECTS:
No adequate evidence for carcinogenicity in humans,
sufficient evidence for carcinogenicity in animals,
IARC classification group 2A (11). BDIV and
Sprague-Dawley rats developed significantly increased
incidence of forestomach tumours following oral
administration (12,13). In skin painting studies mice
showed no increased incidence of skin tumours (14).
GENOTOXICITY: Salmonella typhimurium TA100, TA1535
without metabolic activation positive (31-33).
Salmonella typhimurium TA98, TA1537, TA1538 with and
without metabolic activation negative (31-33).
Saccharomyces cerevisiae mitotic gene conversion
positive (34). Drosophila melanogaster sex-linked
recessive lethal mutations positive (35). In vitro
rat hepatocytes DNA single-strand breaks positive
(...)
/TO TERATOGENICITY AND REPRODUCTIVE EFFECTS: Inhalation
exposure during gestation to 15-100 ppm reduced
fecundity, foetal weight and length in rats and
rabbits and gave rise to ossification defects in

SAMPLE RECORD (cont'd)

rats (9,15,16). Reduced embryonic viability and malformations reported when administered to hens eggs (17,18).

/TO METABOLISM AND TOXICOKINETICS: Detected in the venous blood of workers exposed to styrene (3). Following intraperitoneal injection of styrene to mice the highest concentrations were found in the kidneys, subcutaneous adipose tissue and blood 1-5 hr after administration (19,20). Hydrolysed microsomal epoxide hydrolase from the liver, kidneys, lungs, intestine, and skin of several mammalian species to styrene glycol (21). Other metabolic products include mandelic acid and glutathione conjugates (22,23).
(...)

/TO ADVERSE EFFECTS:
IRRITANCY: Dermal rabbit (24 hr) 10 mg caused well defined erythema and slight oedema (open to the air) (5). Skin irritant in humans (28).
SENSITIZATION: Guinea pig skin sensitised by intradermal injection (29). Caused eye and skin irritation and skin sensitisation in humans (30).
OTHER ADVERSE EFFECTS TO MAN: Inhalation may cause fatigue, headache, weakness, peripheral neuropathy, unsteady gait and central nervous system depression (28).
OTHER ADVERSE EFFECTS: Activities of liver mixed function oxidases and cytochrome P450 content decreased following single intraperitoneal dose of 375 mg kg(-1) body weight to rat (40). Concentrations of 50 and 200 mg kg(-1) body weight in rat decreased liver glutathione content (25).

/DM ENVIRONMENTAL FATE:
ABIOTIC REMOVAL: Waste water treatment: activated carbon adsorbability, 0.19 g g(-1) carbon; 95.3% reduction, influent 1000 mg l(-1), effluent 47 mg l(-1) (4).

/TO OTHER COMMENTS: Genotoxicity reviewed (41,42). Metabolism and pharmacokinetics reviewed (27). Experimental toxicology, human health effects, physico-chemical properties and environmental effects reviewed (43). Autoignition temperature 498 Deg C.

RF= REFERENCES:
1. Pellizzari, E. D. et al Anal. Chem. 1976, 48, 803-807.
2. Sawicki, E. Environmental Pollution and Carcinogenic Risks (INSERM Symposium Series Vol. 52IRC Scientific Publications No. 13) 1976, 315-316, Institut National de la Saute et de la Recherche Medicale, Paris, IARC, Lyon.
(...)
43. ECETOC Technical Report No. 30(5) 1994, European Chemical Industry Ecology and Toxicology Centre, B-1160 Brussels

DP=, /DP DATA PRESENT: Uses; Melting Point; Boiling Point; Vapor Pressure; Density; Partition Coefficient; Solubility; Solubility-Organic; Flash Point; Regulatory; Toxicity; Adverse Effects; Reproductive Effects; Metabolism; Environmental Fate

RD=, PD=, PY= RECORD DATE: 27 Mar 1997

File 307 Dictionary of Substances and Their Effects (DOSE)
SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
— /CN	— CN	All Basic Index Fields Main Substance Name ^{1,2,3}	Word Segment & Word & Phrase	S LYMPHOMA AND BONE(W)Marrow S METHYL/CN S STYRENE(W)OXIDE/CN S STYRENE OXIDE/CN
/DE	DE	Chemical Name ^{1,2,3,4}	Segment & Word & Phrase	S PHENYL(W)ETHANE/NA S EPOXY(1W)PHENYLETHANE/NA S 1,2-EPOXY-1-PHENYLETHANE/NA
/DM	DM	Environmental Fate and Bioaccumulation ⁵	Word	S EFFLUENT/DM S (BOD OR THOD)/DM
/DP	DP	Data Present ^{1,6}	Word	S FLASH(W)POINT/DP
/EC	MF	Element Count ¹	Word	S C8(S)O1/EC
/NA	NA	Chemical Name ^{1,2,3,4}	Segment & Word & Phrase	S PHENYL(W)ETHANE/NA S EPOXY(1W)PHENYLETHANE/NA S 1,2-EPOXY-1-PHENYLETHANE/NA
/OC	OC	Occurrence	Word	S AIR(W)SAMPLE?/OC
/PP	PP	Physical Properties	Word	S LOG(W)POW/PP
/RG	RG	Regulatory Information	Word	S NIOSH(W)NUMBER/RG
/SY	SY	Synonyms ^{1,2,3}	Segment & Word & Phrase	S ETHYLENE/SY S PHENETHYLENE(W)OXIDE/SY S PHENETHYLENE OXIDE/SY
/TO	TO	Toxicity ⁷	Word	S (LD50(5W)RAT)/TO
/US	US	Uses ¹	Word	S (AGROCHEMICALS OR RESINS)/US

¹ Searchable in the Basic Index and in the Additional Indexes.

² All chemical names are searchable as /NA, /DE, or NA=.

³ Chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW to restrict retrieval to the complete term, e.g., S ETHANE/FW to only select ethane as a single word rather than as a segment of a larger chemical term, such as trichloroethane.

⁴ Also /DF.

⁵ Also searchable as /TO; also displays with TO.

⁶ Possible entries for Data Present are: Adverse Effects; Boiling Point; Density; Environment Fate; Flash Point; Melting Point; Metabolism; Partition Coefficient; Regulatory; Reproductive Effects; Solubility; Toxicity; Uses; Vapor Pressure.

⁷ Toxicity field includes Adverse Effects, Reproductive Effects, and Metabolism Effects.

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AA=	AA	Record Identification Number	Phrase	S AA=1359
—	AE	Adverse Effects ⁷		
—	AN	DIALOG Accession Number		
—	AZ	DIALOG Accession Number		
BP=	BP	Boiling Point (Celsius) ^{8,10}	Numeric	S BP=190:200
BT=	BT	Boiling Point Text	Word	S BT=(194 AND DEG)
CN=	CN	Main Substance Name ^{1,2}	Phrase	S CN=STYRENE OXIDE
DN=	DN	Density (Specific Gravity) ^{8,10}	Numeric	S DN=>1.0
DP=	DP	Data Present ^{1,6}	Phrase	S DP=PARTITION COEFFICIENT
DT=	DT	Density Text	Word	S DT=(1(W)0523)
EC=	MF	Element Count ¹	Phrase	S EC=(C0008(S)O0001)
EI=	EI	EINECS/ELINCS Number	Phrase	S EI=202-476-7
FP=	FP	Flash Point (Celsius) ^{8,10}	Numeric	S FP=75:80
FT=	FT	Flash Point Text	Word	S FT=(OPEN(W)CUP)
ME=	MF	Molecular Elements Present	Phrase	S ME=CHO
MF=	MF	Molecular Formula	Phrase	S MF=C8H8O
MP=	MP	Melting Point (Celsius) ^{8,10}	Numeric	S MP=-35.6
MT=	MT	Melting Point Text	Word	S MT=(35(W)6(W)DEG (W)C)
MW=	MW	Molecular Weight ⁸	Numeric	S MW=120.15
NA=	NA	Chemical Name ^{1,2}	Phrase	S NA=PHENYL OXIRANE
NC=	MF	Number of Components	Phrase	S NC=01
NE=	MF	Number of Elements	Phrase	S NE=03
NI=	NI	NIOSH Number	Phrase	S NI= CZ 9625000
OC=	OC	Occurrence	Word	S OC=LATEX
PD=	PD	Record Date ⁹	Phrase	S PD=970327
PI=	PI	Partition Coefficient ^{8,10}	Numeric	S PI=1.61
PT=	PT	Partition Coefficient Text	Word	S PT=(LOG(W)POW(W)1(W)61)
PY=	PY	Publication Year	Phrase	S PY=1997
RD=	RD	Record Date ⁹	Phrase	S RD=27 Mar 1997
RF=	RF	References	Word	S RF=(EUROPEAN(W)CHEMICAL(W)IND?)
RN=	RN	CAS(R) Registry Number	Phrase	S RN=96-09-3
RR=	RR	RTECS Number	Phrase	S RR=CZ9625000
SL=	SL	Solubility	Word	S SL=(ETHANOL AND ACETONE) S SL=(0(W)3)

ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
SY=	SY	Synonyms ^{1,2}	Phrase	S SY=1,2-EPOXY-1-PHENYLETHANE
UD=	—	Update	Phrase	S UD=9999
UN=	UN	UN Number	Phrase	S UN=1114
US=	US	Uses ¹	Word	S US=(TEXTILES OR FIBRES)
VP=	VP	Vapor Pressure (mmHg) ^{8,10}	Numeric	S VP=0.3
VT=	VT	Vapor Pressure Text	Word	S VT=(0(W)3(W)MMHG AND V(W)DEN)

⁸ Numeric values can be entered in several different ways: directly as a number, e.g. S BP=100.0; or in exponential notation, e.g. S BP=1E2. Letter abbreviations are also available: K for thousand; M for million, B for billion, e.g. S BP=0.5K:1.0K. To search a range of values, use a colon between starting and ending values, e.g. S BP=78:79, or use numeric operators (>, <, >=, and <=) e.g. S 78<=BP<=79.

¹⁰ KWIC does not work on the following fields in this database: BP, DN, FP, MP, PI, and VP.

⁹ Record Date, RD=, and Publication Date, PD=, contain the same information, formatted differently.

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

SORT	CN, MF, PD, RN, SY	SORT S4/ALL/RN PRINT S7/9/ALL/CN
RANK	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked.	RANK BP RANK CN S4
MAP	NA, RN, SY	MAP SYRN TEMP S2

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number
2	--	Chemical Names, CAS Registry Number, Molecular Weight, Molecular Formula, Toxicity, Environmental Effect, and Data Present ¹¹
3	Medium	Chemical Names, CAS Registry Number, Physical Properties, and Data Present ¹¹
4	--	Full Record with Tagged Fields
5	Long	Full Record
6	--	Chemical Names
7	--	Chemical Names, CAS Registry Number, Molecular Weight, Molecular Formula, Regulations, and Data Present ¹¹
8	Short	Chemical Names and Data Present
9	Full	Full Record
K	--	KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

¹¹ In the place of a format number, a format name can also be specified to indicate the format, e.g., TYPE S1/TOX/ALL. The Named Formates available are: TOX, PROP, and REG.

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

USER DEFINED FORMATS	User-defined formats may be specified using the display codes indicated in the Search Options tables.	TYPE S4/NA,RN,TO/1-5
TAG	TAG may be used for tagged fields.	TYPE S3/TI,SO/1-5 TAG
DIRECT RECORD ACCESS	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 00199665 DISPLAY 0002789/CO,PC PRINT 0000987/5

FOR ONLINE HELP:

See HELP FIELDS 307 for searchable fields; HELP FORMAT 307 for output formats; HELP LIMIT 307 for limits; HELP RATES 307 for cost information; HELP SORT 307 for sorts.

