iemiscdata: USEPA East Palestine, Ohio Norfolk Southern Train 32N Cargo List – Chemical Databases Match

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Contents

Available Chemical Information

The following provides chemical information from either the chem_wiki or atsdr_tsca_ld50_a data sets from the `chem.databases` R package created by the author for matching chemical substances in the commodities list from the United States Environmental Protection Agency (US EPA) East Palestine, Ohio Norfolk Southern Train 32N Cargo List. The cargo list is one of the data sets in this `iemiscdata` R package also created by the author.

```
install.load::load_package("iemiscdata", "chem.databases", "data.table", "mgsub",
    "stringi", "pander")
# load needed packages using the load_package function from the install.load
# package (it is assumed that you have already installed these packages)

# set the pander options
panderOptions("missing", "")


data(norfolk_southern_epoh)
# from iemiscdata package

data(chem_wiki)
# from chem.databases package

data(atsdr_tsca_ld50_a)
# from chem.databases package



train_commodities <- unique(norfolk_southern_epoh$Commodity)
```

```
pander(train_commodities)
```

POLYPROPYLENE, *POLYETHYLENE*, *residue lube oil*, *VINYL CHLORIDE, STABILIZED* , *DIPROPYLENE GLLYCOL*, *PROPYLENE GLYCOL*, *DIETHYLENE GLYCOL*, *COMBUSTIBLE LIQ., NOS (ETHYLENE GLYCOL MONOBUTYL ETHER)* , *SEMOLINA*, *COMBUSTIBLE LIQ., NOS (ETHYLHEXYL ACRYLATE)* , *POLYVINYL*, *PETROLEUM LUBE OIL*, *POLYPROPYL GLYCOL*, *ISOBUTYLENE*, *BUTYL ACRYLATES, STABILIZED* , *PETRO OIL, NEC* , *ADDITIVES, FUEL* , *BALLS,CTN,MEDCL* , *SHEET STEEL*, *VEGTABLE, FROZEN* , *BENZENE*, *PARAFFIN WAX*, *FLAKES, POWDER* , *HYDRAULIC CEMENT*, *AUTOS PASSENGER* and *MALT LIQUORS*

```
# remove items that are not needed

train_commodities <- train_commodities[-c(3, 9, 16:20, 23:26)]


# remove words that are not needed

train_commodities <- mgsub(train_commodities, c(", STABILIZED", "COMBUSTIBLE LIQ., NOS",
    "LUBE OIL", "WAX"), rep("", 4), fixed = TRUE)


# remove parentheses that are not needed

train_commodities <- mgsub(train_commodities, c("\\(", "\\)"), rep("", 2), fixed = FALSE)


# remove the beginning and trailing white space

train_commodities <- stri_trim_both(train_commodities)


# transform the text to sentence case

train_commodities <- stri_trans_totitle(train_commodities, type = "sentence")


# correct the spelling as needed

train_commodities[4] <- "Dipropylene glycol"

train_commodities[9] <- "Polyvinyl chloride"

train_commodities[13] <- "Butyl acrylate"

pander(train_commodities)
```

Polypropylene, *Polyethylene*, *Vinyl chloride*, *Dipropylene glycol*, *Propylene glycol*, *Diethylene glycol*, *Ethylene glycol monobutyl ether*, *Ethylhexyl acrylate*, *Polyvinyl chloride*, *Petroleum*, *Polypropyl glycol*, *Isobutylene*, *Butyl acrylate*, *Benzene* and *Paraffin*

```
# the exact matched chemical names

pander(chem_wiki[`Substance Name` %in% train_commodities])
```

Table 1: Table continues below

CAS	Substance Name	IUPAC Name	Molecular Formula
9002-86-2	Polyvinyl chloride		
25265-71-8	Dipropylene glycol		C6H14O3
111-46-6	Diethylene glycol	2,2'-Oxydi(ethan-1-ol)	C4H10O3
9003-07-0	Polypropylene		
141-32-2	Butyl acrylate	Butyl prop-2-enoate	C7H12O2
71-43-2	Benzene	Benzene	C6H6
75-01-4	Vinyl chloride	Chloroethene	C2H3Cl

SMILES

C*.C*.OCCOCCO

|lp:4:2,7:2,10:2,m:1:5.6,3:8.9|

OCCOCCO

CCCCOC(=O)C=C

C1=CC=CC=C1

ClC=C

Table 3: Table continues below

InChI

InChI=1S/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2

InChI=1S/C7H12O2/c1-3-5-6-9-7(8)4-2/h4H,2-3,5-6H2,1H3

InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H

InChI=1S/C2H3Cl/c1-2-3/h2H,1H2

Table 4: Table continues below

InChIKey	Average Mass	Monoisotopic Mass
	134.2	134.1
MTHSVFCYNBDYFN-UHFFFAOYSA-N	106.1	106.1
CQEYYJKEWSMYFG-UHFFFAOYSA-N	128.2	128.1
UHOVQNZJYSORNB-UHFFFAOYSA-N	78.11	78.05

BZHJMEDXRYGGRV-UHFFFAOYSA-N 62.5 61.99

```
pander(atsdr_tsca_ld50_a[`Registry Name` %in% train_commodities])
```

CAS	Substance Name	Registry Name	SMILES
111-76-2	Ethanol, 2-butoxy-	Ethylene glycol monobutyl ether	CCCCOCCO
57-55-6	1,2-Propanediol	Propylene glycol	CC(O)CO
71-43-2	Benzene	Benzene	c1ccccc1
75-01-4	Ethene, chloro-	Vinyl chloride	C=CCl
8002-05-9	Petroleum	Petroleum	

```
# the matched names

train_match1 <- chem_wiki[`Substance Name` %in% train_commodities]

train_match2 <- atsdr_tsca_ld50_a[`Registry Name` %in% train_commodities]

train_matchs1 <- train_match1$"Substance Name"

train_matchs2 <- train_match2$"Registry Name"

train_match <- unique(c(train_matchs1, train_matchs2))

pander(train_match)
```

Polyvinyl chloride, *Dipropylene glycol*, *Diethylene glycol*, *Polypropylene*, *Butyl acrylate*, *Benzene*, *Vinyl chloride*, *Ethylene glycol monobutyl ether*, *Propylene glycol* and *Petroleum*

```
train_match_cas1 <- train_match1$CAS

train_match_cas2 <- train_match2$CAS

train_match_cas <- unique(c(train_match_cas1, train_match_cas2))

pander(train_match_cas)
```

9002-86-2, *25265-71-8*, *111-46-6*, *9003-07-0*, *141-32-2*, *71-43-2*, *75-01-4*, *111-76-2*, *57-55-6* and *8002-05-9*

```
# remove the matched names

train_commodities2 <- train_commodities[-which(train_commodities %in% train_match)]


# these are the chemical substances without an exact match

pander(train_commodities2)
```

Polyethylene, *Ethylhexyl acrylate*, *Polypropyl glycol*, *Isobutylene* and *Paraffin*

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