

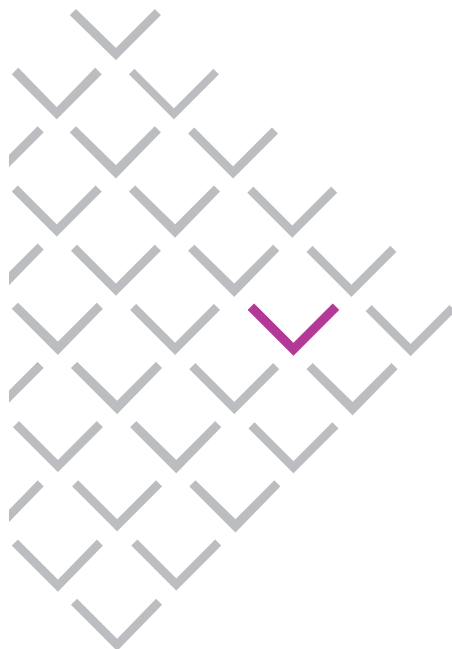


Chemical Abstracts Service
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in North America

STNNotes

JULY 1995

No. 6



CAS Registry Enhancement

*Structure and other access
points to polymer esters
and ethers and indefinite
nonpolymeric esters*

**You can now search
not only names but
also structures, molecular
formulas, component
Registry Numbers,
and other fields for
the following classes
of substances in Registry:**

- **polymer esters**
- **polymer ethers**
- **nonpolymeric esters
with unknown
positions and numbers
of ester groups**

In response to customer requests for more detailed information on new and enhanced system features, we have created STNNotes. STNNotes give you the in-depth technical details you need for efficient use of STN. We hope you find this information useful. Please let us know how we can continue to improve in meeting your technical information needs.

Until May 1995 polymer esters, polymer ethers, and indefinite nonpolymeric esters were "manually" registered in the CAS Registry File. Because of the indefinite nature of their structures, they were assigned only CAS Registry Numbers and the CA index names, so you could not search them in other ways. Structure-based registration of new polymer esters, ethers, and indefinite nonpolymeric esters began in mid-May 1995. Conversion of existing manual registrations to structural representation also has begun and will continue over a period of time as the backfile is gradually processed.

In the Registry File, there are about 15,000 - 20,000 polymer esters and ethers. These compounds are now being upgraded to structural representations as dot-disconnected components consisting of the base polymer and the ester- or ether-forming agent standardized to its free acid or alcohol form. Some of the polymer types that are affected by this

upgraded registration include the following:

- **monomer-based polymer esters and ethers, e.g., alkylene oxide homo- and copolymer esters and ethers, acrylic polymer esters, caprolactone homopolymer esters, epoxy resin esters**
- **structural repeating unit (SRU) esters and ethers, e.g., polyalkylene glycol SRU esters and ethers, with an indefinite number of ester or ether groups**
- **natural polymer esters and ethers, e.g., cellulose esters and ethers, polysaccharide esters and ethers, polynucleotide esters**

There are approximately 9,000 nonpolymeric esters with unknown positions and numbers of ester groups. These registrations are also being upgraded to structure-based registrations using dot-disconnected free acid and alcohol components.

As the examples illustrate, you can now search these compounds using not only names but also

- **molecular formula for each component and the entire compound**
- **structure for each component and the entire compound**
- **CAS Registry Number for each component**

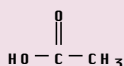
In addition, you can use polymer class terms to search polymer esters and ethers.

Current Record for a Polymer Ester

RN 71714-39-1 REGISTRY
 CN Furan, tetrahydro-, homopolymer, diacetate (9CI) (CA INDEX NAME)
 DR 72270-49-6
 MF (C4 H8 O)x . 2 C2 H4 O2
 PCT Polyether, Polyether formed
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
 DES 8:GD,ESTER

CM 1

CRN 64-19-7
 CMF C2 H4 O2



CM 2

CRN 24979-97-3
 CMF (C4 H8 O)x
 CCI PMS

CM 3

CRN 109-99-9
 CMF C4 H8 O



4 REFERENCES IN FILE CA (1967 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

New search and display data: molecular formula and structure for each component, CAS Registry Number for each component (CRN), and polymer class terms (PCT).

Previous Record for a Polymer Ester

RN 71714-39-1 REGISTRY
 CN Furan, tetrahydro-, homopolymer, diacetate (9CI) (CA INDEX NAME)
 DR 72270-49-6
 MF Unspecified
 CI PMS, MAN
 PCT Manual registration
 LC STN Files: CA, IFICDB, IFIPAT, IFIUDB, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

4 REFERENCES IN FILE CA (1967 TO DATE)

New search and display data: molecular formula and structure for each component, CAS Registry Number for each component (CRN), and polymer class terms (PCT).

Current Record for a Polymer Ether

RN 9065-63-8 REGISTRY
 CN Oxirane, methyl-, polymer with oxirane, butyl ether (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Oxirane, polymer with methyloxirane, butyl ether (9CI)
 OTHER NAMES:
 CN Ethylene oxide-propylene oxide polymer butyl ether
 CN Polyoxyethylene polyoxypropylene butyl ether
 DR 52519-69-4, 39465-06-0, 9050-72-0
 MF C₄H₁₀O . x (C₃H₆O . C₂H₄O)_x
 CI COM
 PCT Polyether, Polyether formed
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXLIT, USPATFULL
 DES 8:GD,ETHER

CM 1

CRN 71-36-3
 CMF C₄H₁₀O

H₃C-CH₂-CH₂-CH₂-OH

CM 2

CRN 9003-11-6
 CMF (C₃H₆O . C₂H₄O)_x
 CCI PMS

CM 3

CRN 75-56-9
 CMF C₃H₆O



CM 4

CRN 75-21-8
 CMF C₂H₄O



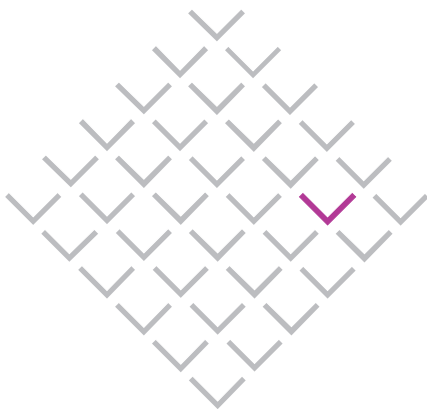
59 REFERENCES IN FILE CA (1967 to DATE)
 7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 59 REFERENCES IN FILE CAPLUS (1967 to DATE)

Previous Record for a Polymer Ether

RN 9065-63-8 REGISTRY
 CN Oxirane, methyl-, polymer with oxirane, butyl ether (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Oxirane, polymer with methyloxirane, butyl ether (9CI)
 OTHER NAMES:
 CN Ethylene oxide-propylene oxide polymer butyl ether
 CN Polyoxyethylene polyoxypropylene butyl ether
 DR 52519-69-4, 39465-06-0, 9050-72-0
 MF Unspecified
 CI PMS, COM, MAN
 PCT Manual registration
 LC STN Files: CA, IFICDB, IFIPAT, IFIUDB, TOXLIT, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

59 REFERENCES IN FILE CA (1967 to DATE)
 7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

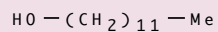


Current Record for a Nonpolymeric Ester

RN 55762-75-9 REGISTRY
CN Butanedioic acid, dodecyl ester (9CI) (CA
INDEX NAME) OTHER NAMES:
CN Dodecyl succinate
MF C12 H26 O . x C4 H6 O4
LC STN Files: CA, CAPLUS
DES 8:GD,ESTER

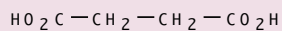
CM 1

CRN 112-53-8
CMF C12 H26 O



CM 2

CRN 110-15-6
CMF C4 H6 O4



3 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

**New search and
display data:
molecular
formula and
structure for
each component,
and CAS Registry
Number for each
component (CRN).**

Previous Record for a Nonpolymeric Ester

RN 55762-75-9 REGISTRY
CN Butanedioic acid, dodecyl ester (9CI)
(CA INDEX NAME) OTHER NAMES:
CN Dodecyl succinate
MF Unspecified
CI MAN
LC STN Files: CA

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

3 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA