EASTMAN

Building blocks for better resins

DMCD

Contents

Product. Innovation. Support. Commitment.

You spend a lot of time and energy developing resins that meet stringent demands. Eastman resin intermediates are the building blocks that make those resins even better. Eastman products serve the resins market for coatings, fiberglass reinforced plastics, gel coats, adhesives and inks applications.

With more than 60 years of experience in this industry, Eastman has developed intermediates that help meet your performance needs.

Not only do you need the right building blocks to develop resins, but you also need adequate support behind them. We stand behind our products with innovative and proven technical and business support. Our teams of sales, business and technical personnel can help with your business opportunities and product development.

The right combination of products and people creates a winning solution. Eastman doesn't just make the building blocks for better resins. We also build blocks for better business.

Proven performance

Eastman has one of the broadest product lines of any raw material supplier. Available intermediates include aromatics, cycloaliphatics and neostructures.

Our product line includes such workhorses as Eastman NPG glycol. Our specialty intermediates meet stringent regulatory, performance and testing demands for coatings and composites applications.

Since resin performance is related to the intermediate used, an understanding of the structural features and performance characteristics of the intermediate is the first step in designing resins to meet specific needs. An intermediate typically performs similarly across applications.

This publication describes the structural features and expected performance characteristics of Eastman intermediates. Synthesis tips are also provided for each intermediate, as well as typical properties and regulatory clearances.

The foundation for Eastman resin intermediates

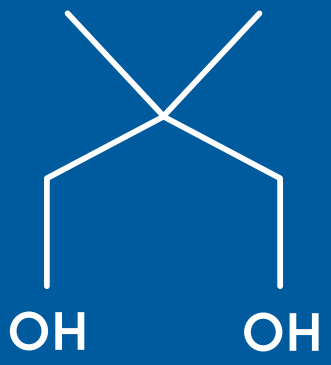
Neostructures

- Eastman NPG glycol — 2,2-dimethyl-1, 3-propanediol
- Eastman TMPD glycol — 2,2,4-trimethyl-1, 3-pentanediol

Cycloaliphatics

- 1,4-CHDA HP — 1,4-cyclohexanedicarboxylic acid
- CHDM-D — 1,4-cyclohexanedimethanol
- DMCD — dimethyl-1,4-cyclohexane dicarboxylate

Glycols
Eastman NPG glycol
(2,2-dimethyl-1,3-propanediol)



IUPAC: 2,2-dimethyl-1,3-propanediol

Structure/property relationships

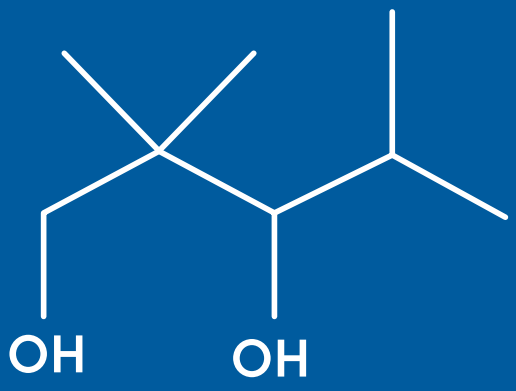
Structural features	Performance characteristics
Absence of beta hydrogens	Excellent weatherability
Primary hydroxyl groups	Rapid reactivity during esterification and cure
Slightly hindered hydroxyl groups	Good humidity resistance Good corrosion resistance Good chemical resistance Good stain resistance
Symmetrical	Excellent thermal stability for low resin color Moderate solution viscosity High T_g
Pendant methyl groups	Good solubility

Synthesis tips

- Water solubility and sublimation of Eastman NPG glycol make a packed, partial-condensing column desirable.
- Good thermal stability gives low-color resins even at synthesis temperatures of 240°–250°C.
- Two primary hydroxyls offer good reactivity.
- Although an esterification catalyst is not required when reacting with many acid functional intermediates, 0.1 wt% monobutyltin oxide based on total reactor charge can reduce processing time.
- When transesterifying Eastman NPG glycol with an ester such as DMCD, use 0.1 wt% PTSA (p-toluenesulfonic acid monohydrate) based on total reactor charge to stabilize the glycol.

Eastman TMPD glycol

(2,2,4-trimethyl-1,3-pentanediol)



IUPAC: 2,2,4-trimethyl-1,3-pentanediol

Structure/property relationships

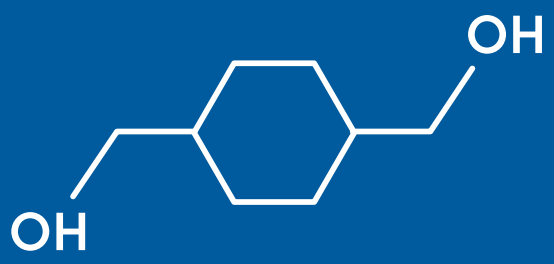
Structural features	Performance characteristics
Bulky, asymmetrical	Low solution viscosity Low resin density Excellent solubility
Sterically hindered hydroxyl groups	Excellent resin hydrolytic stability Excellent chemical resistance Excellent stain resistance Good humidity resistance Good corrosion resistance Moderate reactivity during esterification and cure
Branched chain	Moderate thermal stability Low T_g
Beta hydrogens	Moderate weatherability

Synthesis tips

- Water insolubility makes a packed column unnecessary unless used in combination with other water-soluble glycols.
- 0.1 wt% monobutyltin oxide based on total reactor charge will help esterify the secondary hydroxyl.
- Avoid rapid heating. Hold reaction temperature between 180°–200°C during first 30%–60% of reaction. Limit reaction temperature to a maximum of 215°C.
- For processing Eastman TMPD glycol with anhydrides, consider the following options:
  - Stage either the anhydride or TMPD glycol with other reactants.
  - Do not charge anhydride initially with TMPD glycol; add anhydride to molten TMPD glycol.
  - Use a process solvent, such as 3–7 wt% xylene based on total reactor charge.

CHDM glycol

(1,4-cyclohexanedimethanol)



IUPAC: 1,4-cyclohexanedimethanol

Structure/property relationships

Structural features	Performance characteristics
Absence of beta hydrogens	Excellent weatherability
Primary hydroxyl groups	Rapid reactivity during esterification and cure
Slightly hindered hydroxyl groups	Good humidity resistance Good corrosion resistance Good chemical resistance Good stain resistance
Symmetrical	Excellent thermal stability for low resin color Moderate solution viscosity High T_g
Pendant methyl groups	Good solubility

Synthesis tips

- To ensure a uniform mixture of isomers, melt entire contents of CHDM container and agitate prior to using.
- Use CHDM as a partial replacement for Eastman NPG glycol or other glycol intermediates.
- Water solubility makes a packed, partial-condensing column desirable.
- Good thermal stability yields low-color resins even at synthesis temperatures of 240°–250°C.
- Two primary hydroxyls offer excellent reactivity and reduced synthesis times.
- Although an esterification catalyst is not required when reacting with many acid functional intermediates, 0.1 wt% monobutyltin oxide based on total reactor charge can reduce processing times.

Diacids and diesters
1,4-CHDA
(1,4-cyclohexanedicarboxylic acid)

IUPAC: 1,4-cyclohexanedicarboxylic acid

Structure/property relationships

Structural features	Performance characteristics
Saturated ring	• Excellent solubility in molten glycols for rapid processing • Excellent resin hydrolytic stability • Excellent thermal stability for low resin color • Excellent combination of hardness and flexibility • Improved corrosion and stain resistance compared to linear aliphatic acids • Excellent weathering in gel coats • Moderate weathering in unstabilized coatings • Excellent weathering in stabilized coatings • Good humidity resistance
1,4-substitution	Moderate resin solubility

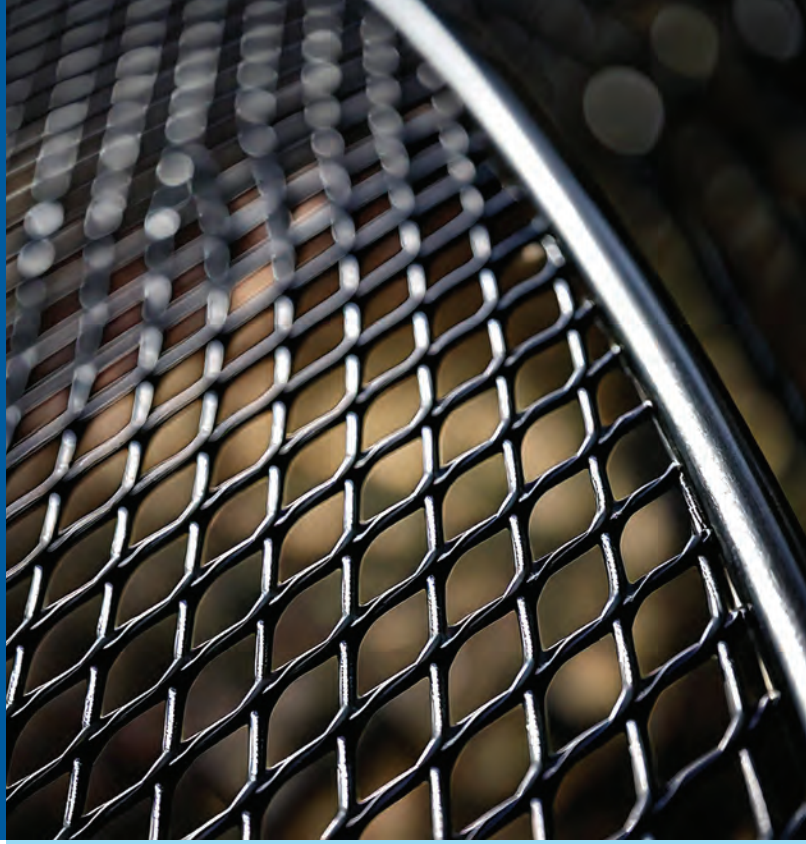
Synthesis tips

- Having good thermal stability results in low-color resins, even at high synthesis temperatures (240°–250°C).
- Saturated ring structure gives excellent solubility and rapid synthesis in molten glycols, even at temperatures of 90°–200°C.
- An esterification catalyst is not required, but 0.1 wt% monobutyltin oxide based on total reactor charge can reduce process times.

DMCD

(Dimethyl 1,4-cyclohexanedicarboxylate)

UPAC: Dimethyl 1,4-cyclohexanedicarboxylate



Structure/property relationships

Structural features	Performance characteristics
Bulky, asymmetrical	Low solution viscosity Low resin density Excellent solubility
Sterically hindered hydroxyl groups	Excellent resin hydrolytic stability Excellent chemical resistance Excellent stain resistance Good humidity resistance Good corrosion resistance Moderate reactivity during esterification and cure
Branched chain	Moderate thermal stability Low T_g
Beta hydrogens	Moderate weatherability

Synthesis tips

- Water insolubility makes a packed column unnecessary unless used in combination with other water-soluble glycols.
- 0.1 wt% monobutyltin oxide based on total reactor charge will aid in the esterification of the secondary hydroxyl.
- Avoid rapid heating. Hold reaction temperature between 180°–200°C during first 30%–60% of reaction. Limit reaction temperature to a maximum of 215°C.
- For processing Eastman TMPD glycol with anhydrides, consider the following options:
  - Stage either the anhydride or TMPD glycol with other reactants.
  - Do not charge anhydride initially with TMPD glycol; add anhydride to molten TMPD glycol.
  - Use a process solvent, such as 3–7 wt% xylene based on total reactor charge.

Product summary

Performance benefits

	Glycol			Diacid/diester	
	Eastman NPG glycol	Eastman TMPD glycol	CHDM	CHDA	DMCD
Resin					
Processibility	●		●	●	
Thermal stability	●		●	●	●
Low color	●	●	●	●	●
Low solution viscosity		●			
Hydrolytic stability		●		●	●
Coating/composite					
Hardness	●	●	●	●	●
Flexibility	●			●	●
Stain resistance	●	●			
Corrosion resistance	●	●	●	●	●
Chemical resistance	●	●	●	●	●
Humidity resistance	●	●	●	●	●
Excellent weathering	●		●	●	●

Technology and application

	Glycol			Diacid/diester	
	Eastman NPG glycol	Eastman TMPD glycol	CHDM	CHDA	DMCD
Technology					
High solids	●	●	●	●	●
Powder	●		●	●	
Waterborne	●	●	●	●	
Radiation cure	●	●	●	●	●
Conventional	●		●	●	●
Application					
Auto OEM	●	●	●	●	●
Auto refinish	●	●	●	●	●
Industrial maintenance	●	●	●	●	●
Coil	●		●	●	
Appliance	●	●	●	●	●
Metal furniture	●	●	●	●	●
Container	●		●	●	●
Heat sensitive substrates	●	●	●	●	●
FRP	●	●	●	●	●
Gel coats	●	●	●	●	
Corrosion resistant resins	●	●			

Typical properties

Product	Physical form	Molecular weight	Equivalent weight	Assay, wt%	Melting point, °C
Eastman NPG glycol	Platelets molten	104.15	52.07	99.2	124–130
Eastman NPG 90 glycol	Liquid[a]	104.15	52.07	89	31[a]
Eastman TMPD glycol	Solid waxy platelets molten	146.22	73.11	98.2	46–55
CHDM-D[b]	Solid molten	144.21	72.11	98.5	41–61
CHDM-D90[b]	Liquid	144.21	72.11	88	-30–+40
1,4-CHDA[b]	Powder	172.00	86.00	99	164–167
DMCD[b]	Slurry molten	200.23	100.12	93	14 (cis) 71 (trans)

Product	Boiling point, °C	Specific gravity, 20°/20°C	Solubility in water, wt% at 20°C unless noted	Wt% solids	Volatile
Eastman NPG glycol	210	1.06	84 (25°C)	100	None
Eastman NPG 90 glycol	100–121	0.94 (60°C)	—	90	Water
Eastman TMPD glycol	220–235	0.928 (55°/15°C)	3.6	100	None
CHDM-D[b]	284–288	1.02	47.9	100	None
CHDM-D90[b]	113	0.95	—	90	Water
1,4-CHDA[b]	—	1.38	1	100	None
DMCD[b]	259	1.102 (35°/4°C)	1.2 (25°C)	100	None

[a]Crystallizes below 31°C
[b]Mixture of cis/transisomers
[c]Sublimes
[d]Cross-linker dependent
[e]Extrapolated under vacuum

Eastman resin intermediates are available in bulk and various package sizes. Contact Eastman technical service or your Eastman sales representative for packaging options and availability.

CHDM-D90 is a CHDM-D/water mixture exhibiting multiple melting points across this range. This complexity makes melting and freezing point determinations difficult.
Eastman suggests CHDM-D90 be stored and handled at temperatures between -30 and 40°C.

Regulatory information

Resin intermediate	CAS registry number[a]	FDA clearance (U.S.)[b,c]	Directive 2002/72/ EC (Europe)[c,d]	TSCA (U.S.)[e]
1,4-CHDA	1076-97-7	21 CFR 175.300(b)(3)(vii)(a)	Listed	Listed
CHDM-D and/or CHDM-D90[k]	105-08-8	21 CFR 175.105 21 CFR 175.300 (FCN 87)[l] 21 CFR 177.1680	Listed	Listed
DMCD	94-60-0	21 CFR 175.105	Not listed	Listed
Eastman NPG glycol and/or Eastman NPG 90 glycol[k]	126-30-7	21 CFR 175.105 21 CFR 175.260 21 CFR 175.300(b)(3)(vii)[l] 21 CFR 175.300(b)(3)(xxxvii) 21 CFR 175.320 21 CFR 177.1680 21 CFR 177.2420	Listed	Listed
Eastman TMPD glycol (platelets and molten)	Liquid	21 CFR 177.2420	Not listed	Listed

Resin intermediate	EINECS number (Europe)[f]	DSL (Canada)[g]	AICS/ NICNAS (Australia)[h]	MITI (Japan)[i]	ECL (Korea)[j]
1,4-CHDA	214-068-6	Listed	Listed	Listed	Listed
CHDM-D and/or CHDM-D90[k]	203-268-9	Listed	Listed	Listed	Listed
DMCD	202-347-5	Listed	Listed	Listed	Not listed
Eastman NPG glycol and/or Eastman NPG 90 glycol[k]	204-781-0	Listed	Listed	Listed	Listed
Eastman TMPD glycol (platelets and molten)	205-619-1	Listed	Listed	Listed	Listed

[a] Chemical Abstract Services
[b] In addition to the above listings, there are additional FDA regulations and food contact notifications for specific polymer compositions that utilize one or more of these monomers.
[c] In all cases, the applicable food-contact regulations or listings must be consulted to determine the applicable restrictions on use in contact with food.
[d] Commission Directive 2002/72/EC relating to plastic materials and articles intended to come into contact with foodstuff.
[e] U.S. Toxic Substances Control Act
[f] European Inventory of Existing Commercial Chemical Substances
[g] Canadian Domestic Substances List
[h] Australian Inventory of Chemical Substances and National Industrial Chemicals Notification and Assessment Scheme
[i] Japanese Handbook of Existing and New Chemical Substances
[j] Korean Toxic Substances Control Act
[k] Contains 10% water; CAS registry number for water is 7732-18-5.
[l] Polyesters regulated at 21 CFR 175.300 are also referenced for use in various other regulations including 21 CFR 176.170(b)(1) and 21 CFR 177 1210(b). Use is subject to the limitations of applicable regulations for the intended use.

Technical solutions

Technical service

Eastman's technical service laboratory has the expertise and capabilities to help you develop resins for various coatings and composites. Our strength is in understanding the performance benefits of resin intermediates relative to their structure/property relationships.

We can help you select the right building blocks to meet resin performance requirements and understand how to properly use them. We have developed an extensive list of "synthesis tips" that facilitate resin processing with Eastman resin intermediates.

Our automated resin synthesis methods put us on the leading edge of resin processing capabilities. We share our experience in this with customers. Automation's advantages include reducing operator variability, improving batch-to-batch consistency, increasing efficiency and enhancing data collection and analysis for the study of resin reaction profiles.

In addition to resin formulation and processing, we have the expertise to formulate, apply and evaluate resins in coatings systems, fiberglass-reinforced plastics, and gel coats. We can perform the tests that have become standard in the coatings and composites industries. Testing is performed on resins, coatings, cured films, castings, laminates and gel coats. Moreover, we have invested in a state-of-the-art powder-coating processing, application and test facility to support customer development of this growing technology area.

Under the Responsible Care® pledge, Eastman is committed to protecting the health and safety of people and the environment. Product stewardship is an important initiative of Responsible Care® that ensures the proper use and handling of Eastman products by chemical manufacturers and distributors throughout product lifecycles. The product stewardship carried out in the technical service resin intermediates laboratory helps customers safely handle and use Eastman products.

Eastman technical service can assist you in resin design, laboratory resin synthesis, production scale-up, coating and composites formulation, and product stewardship issues. Contact an Eastman representative about designing high-performance resins with Eastman resin intermediates.

► *Computer control for automated resin synthesis*

Polyester Resin Calculation Wizard

The Polyester Resin Calculation Wizard is a novel approach to resin design and the understanding of resin processing. It calculates resins for coatings, inks and adhesives applications. Selecting raw materials and entering certain resin parameters will produce a reactor charge, process logs and graphical representations of the theoretical polymerization data. The results are printable or downloadable.

Benefits

- More advanced features and easier to use than other industry tools
- Graphs visually represent polymerization and help anticipate gel points.
- Process logs provide guidance during resin processing with respect to changes in acid number, hydroxyl number, molecular weight and evolved distillate.
- Generates resin properties at desired acid or hydroxyl number
- Reactor charge is easily scaled for laboratory, pilot and plant batches.
- Results are printed in a logical, easy-to-read, ready-to-use format. They can also be downloaded or emailed.
- Standardizes resin calculations performed within a company
- Links to Eastman resin intermediate product pages are available for additional information.
- Connect to Eastman technical service representatives

To access the polyester resin calculator, visit eastman.com/resinwizard.

Building blocks on eastman.com

For more information at your fingertips, visit **eastman.com/resinintermediates.**

Information on this website includes:

- Product information
- Technical publications
- Contact information for technical service
- Wizard access

EASTMAN

Eastman Corporate Headquarters
P.O. Box 431
Kingsport, TN 37662-5280 U.S.A.

U.S.A. and Canada, 800-EASTMAN (800-327-8626)
Other locations, +(1) 423-229-2000

eastman.com/locations

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