Product Information:
Product: 3-Chloroperoxybenzoic acid, 70-75%
Synonym: m-Chloroperoxybenzoic acid; m-CPBA; MCPBA
Acros code number: 25579-0000
CAS number: 937-14-4
EINECS number: 213-322-3
TSCA: listed
MDL code number: MFCD00002127
Structure:

\[
\begin{align*}
\text{O} & \text{O} \\
\text{OH} & \\
\text{Cl} & \\
\text{C}_7\text{H}_5\text{ClO}_3 & \\
\end{align*}
\]

Molecular formula: C7H5ClO3
Molecular weight: 172.57 g/mol

Specifications:
Appearance: White moist powder
Assay Iodometry: 70 to 75%
3-Chlorobenzoic acid: ≤12%
Water: (K.F.) balance
Separat. Techn. HPLC: ≤0.2% Di-m-chlorobenzoyl peroxide
≤0.1% sec-Butanol

Typical Properties:
Odor: slight pungent odor
Melting point: 92-94 °C
SADT: 55 °C (Self-Accelerating Decomposition Temp.)
Decomposition: >88 °C
Major decomposition products: 3-Chlorobenzoic acid, Water
Bulk density: 0.56 g/cm³
pH saturated aq. sol.: 4.5 @ 25 °C
pKa: 7.57 (in water @ 25 °C)
Solubility[^1][^136]:
- Water: 0.154 g/100 ml
- Hexane: 1.4 g/100 ml
- CCl₄: 2.1 g/100 ml
- Benzene: 8.0 g/100 ml
- Chloroform: 9.8 g/100 ml
- CH₂Cl₂: 11.2 g/100 ml
- Ethyl acetate: 51.0 g/100 ml
- tert-Butanol: 69.0 g/100 ml
- Diethyl ether: 89.4 g/100 ml
- Ethanol: 113.0 g/100 ml
General Information: 3-Chloroperoxybenzoic acid (MCPBA) is one of the most popular oxidation reagent in organic synthesis, because of its outstanding performance in terms of:
- reactivity, combined with reducing the number of reaction steps in classical synthetic routes,
- regio- and stereoselectivity,
- protection of functional groups mostly not required,
- high purity and yields.
Its literature covers a huge area of different syntheses and below reaction equations just can be a brief overview of its interesting applications:

1. Epoxidation:\(^1,^2,^3,^4,^5,^6:\)

\[
\begin{align*}
R\equiv C\equiv C\equiv R''' & \quad \xrightarrow{\text{MCPBA}} \quad R\equiv C\equiv C\equiv R'''
\end{align*}
\]

2. Baeyer-Villiger Oxidation:\(^7,^8,^9:\)

\[
\begin{align*}
\text{O} & \quad \xrightarrow{\text{MCPBA}} \quad \text{O}
\end{align*}
\]

3. Synthesis of Sulfoxides & Sulfones:\(^10,^11,^12,^13:\)

\[
\begin{align*}
R\equiv S\equiv R' & \quad \xrightarrow{\text{MCPBA}} \quad \text{S}
\end{align*}
\]

4. Synthesis of N-Oxides with tertiary amines:\(^14,^15,^16:\)

\[
\begin{align*}
R\equiv N \equiv R'' & \quad \xrightarrow{\text{MCPBA}} \quad R\equiv N \equiv R''
\end{align*}
\]

5. Synthesis of Nitro compounds with prim. Amines:\(^17:\)

\[
\begin{align*}
R\equiv \text{NH}_2 & \quad \xrightarrow{\text{MCPBA}} \quad R\equiv \text{NO}_2
\end{align*}
\]

6. Conversion of Aziridines to Olefins:\(^18:\)

\[
\begin{align*}
\text{N} & \quad \xrightarrow{\text{MCPBA}} \quad \text{N}
\end{align*}
\]

7. Oxidation of Imino ethers to esters and hydroxylamines:\(^19:\)

\[
\begin{align*}
\text{H} \equiv C \equiv \text{O} \equiv R' & \quad \xrightarrow{\text{MCPBA}} \quad \text{H} \equiv C \equiv \text{O} \equiv R' \\
\text{H} \equiv C \equiv \text{O} \equiv R' & \quad \xrightarrow{\text{H}^+} \quad \text{HCOOR'} + \text{RNHOH'}
\end{align*}
\]

8. Synthesis of Aldehydes and Acids with α-Hydroxy ketones:\(^20:\)

\[
\begin{align*}
\text{R} \equiv C \equiv \text{C} \equiv \text{R'} & \quad \xrightarrow{\text{MCPBA}} \quad \text{R} \equiv C \equiv \text{C} \equiv \text{R'} \\
\text{R} \equiv C \equiv \text{C} \equiv \text{R'} & \quad \xrightarrow{\text{RCHO} + \text{RCOOH}}
\end{align*}
\]
9. Synthesis of Alcohols with primary Alkyl iodides\textsuperscript{21}:

\[
\begin{array}{c}
R\underset{\text{MCPBA}}{\rightarrow} R\text{-OH}
\end{array}
\]

Handling and Storage: Use only under a chemical fume hood. Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Do not breathe vapor/dust. Do not ingest. Keep containers tightly closed in a dry, cool and well-ventilated place. Do not store near combustible materials. Keep refrigerated (@ approx. +2 to +8 °C). Organic peroxides.

Material Safety Data Sheet: A Material Safety Data Sheet (MSDS) according to EU guideline 91/155/EWG can be downloaded from our website http://www.acros.com

Packaging: Bulk: 25 kg HDPE plastic drum. Prepack: HDPE plastic containers in: 25g, 100g, 500g, and 1kg.

Transport regulations: UN-Number: 3106
ADR: Hazard Class: 5.2
Packaging Group: II
IMDG: Hazard Class: 5.2
Packaging Group: II
IATA: Hazard Class: 5.2
Packaging Group: II

Literature: Fieser: 1, 135; 2, 68; 3, 49; 4, 85; 5, 120; 6, 110; 7, 62; 8, 97; 9, 108; 10, 92; 11, 122; 12, 118; 13, 76; 15, 86; 16, 80; 17, 76.

Note:
The information submitted in this publication is based on our current knowledge and experience. In view of the many factors that may affect processing and application, these data do not relieve processors of the responsibility of carrying out their own tests and experiments. Neither do they imply any legally binding assurance of certain properties or of suitability for a specific purpose. It is the responsibility of those to whom we supply our products to ensure that any proprietary rights and existing laws and legislation are observed.