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Technical Data Sheet Catalog Number: C40770

For research use only

Not intended or approved for diagnostic or therapeutic use.

## Product Name: Chlorin e6 trimethyl ester

Catalog Number: C40770



Sizes Available: 100 mg, 250 mg , 500 mg, 1.0 g, 5.0 g, 10.0 g available, Bulk pricing available

Molecular weight: 638.8 g/mol

Molecular Formula: C<sub>37</sub>H<sub>42</sub>N<sub>4</sub>O<sub>6</sub>

**CAS Number:** 35038-32-5

Storage: Store at room temperature, protect from light

**Synonyms:** Chlorin-e6-trimethyl ester, Methyl (2S-trans)-13-ethyl-2,3-dihydro-18-(methoxycarbonyl)-20-(2-methoxy-2-oxoethyl)-3,7,12,17-tetramethyl-8-vinyl-21H,23Hporphine-2-propionate, Chlorine e6, trimethyl ester, EINECS 252-329-6, NSC75785, NSC-75785

## Field of Interest: Natural Products Synthesis, Photodynamic Therapy, Photophysics

**Background: Chlorin e6 trimethyl ester** Is active as a photosensitizing agent in photodynamic therapy and a well studied compound by R. B. Woodward, elaborating synthesis of chlorins and compounds related to chlorophyll <sup>1,2</sup> Metallation and reactions of the ring system are extensively studied,<sup>3</sup> and the mono L- aspartylchlorin-e6 analog is known as Talaporfin, an important clinical agent.<sup>4</sup>

## **References:**

- 1) Pandey, Ravindra K.; Bellnier, David A.; Smith, Kevin M.; Dougherty, Thomas J., Chlorin and porphyrin derivatives as potential photosensitizers in photodynamic therapy. Photochemistry and Photobiology (1991), 53(1), 65-72.
- Woodward, R. B.; Skaric, Vinko, A new aspect of the chemistry of chlorins, Journal of the American Chemical Society (1961), 83, 4676-8. And Woodward, R. B.; Ayer, W. A.; Beaton, J. M.; Bickelhaupt, F.; Bonnett, R.; Buchschacher, P.; Closs, G. L.; Dutler, H.; Hannah, J.; Hauck, F. P.; et al. The total synthesis of chlorophyll, Journal of the American Chemical Society (1960), 82, 3800-2. DOI:10.1021/ja01499a093.
- O'Shea, Donal F.; Miller, Mark A.; Matsueda, Hiroko; Lindsey, Jonathan S., In, vestigation of the Scope of Heterogeneous and Homogeneous Procedures for Preparing Magnesium Chelates of Porphyrins, Hydroporphyrins, and Phthalocyanines, Inorganic Chemistry (1996), 35(25), 7325-7338. DOI:10.1021/IC960812P
- 4) Hargus, Jodie A.; Fronczek, Frank R.; Vicente, M. Graca H.; Smith, Kevin M., Mono-(L)aspartylchlorin-e6, Photochemistry and Photobiology (2007), 83(5), 1006-1015. DOI:10.1111/j.1751-1097.2007.00092.x

**Hazardous Properties and Cautions:** The toxicological and pharmacological properties of this compound are not fully known. For further information see the SDS on request. **Chlorin e6 trimethyl ester** is manufactured, shipped according to standard practices, and intended for research and development in a laboratory utilizing prudent procedures for handling chemicals of unknown toxicity, under the supervision of persons technically qualified to evaluate potential risks and authorized to enforce appropriate health and safety measures. As with all research chemicals, precautions should be taken to avoid unnecessary exposures or risks.

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