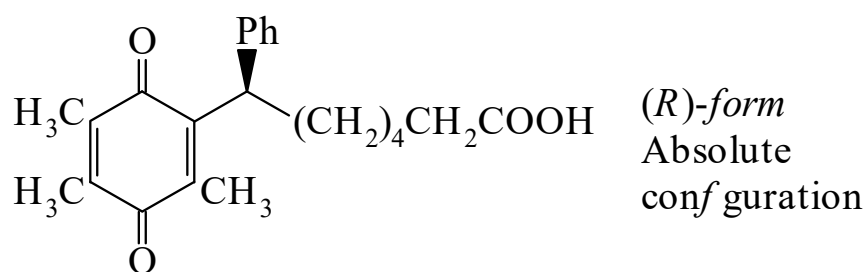




>>Entry Name: Seratrodast, INN

Synonym(s): ξ -(2,4,5-Trimethyl-3,6-dioxo-1,4-cyclohexadien-1-yl)benzeneheptanoic acid, 9Cl. 7-(3,5,6-Trimethyl-1,4-benzoquinon-2-yl)-7-phenylheptanoic acid. Serabenast. Bronica. AA 2414. Abbott 73001



CAS Registry Number: 103186-19-2

Related CAS Registry Numbers(s): 103187-07-1

Molecular Formula: C₂₂H₂₆O₄

Molecular Weight: 354.445

Accurate Mass: 354.18311

Percentage Composition: C 74.55%; H 7.39%; O 18.06%

Use/Importance: Thromboxane A₂-receptor antagonist. Bronchodilator, antiasthmatic agent

Development Status: Awaiting approval for clinical use in Japan (1996)

>>Variant: (R)-form

CAS Registry Number: 103187-09-3

Molecular Formula: C₂₂H₂₆O₄

Molecular Weight: 354.445

Accurate Mass: 354.18311

Percentage Composition: C 74.55%; H 7.39%; O 18.06%

Physical Description: Cryst. (diisopropyl ether)

Melting Point: Mp 77-80°

Optical Rotation: [α]_D +24.8 (c, 1.0 in CHCl₃) (96% ee)

Other Data: More potent isomer

>>Variant: (S)-form

CAS Registry Number: 103196-89-0

Molecular Formula: C₂₂H₂₆O₄

Molecular Weight: 354.445

Accurate Mass: 354.18311

Percentage Composition: C 74.55%; H 7.39%; O 18.06%

Optical Rotation: [α]_D -24.8 (c, 1.0 in CHCl₃) (96% ee)

>>Variant: (±)-form

CAS Registry Number: 112665-43-7

Molecular Formula: C₂₂H₂₆O₄

Molecular Weight: 354.445

Accurate Mass: 354.18311

Percentage Composition: C 74.55%; H 7.39%; O 18.06%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 128-129°

References:

- Eur. Pat.*, 1987, *Takeda*, 232 089; *CA*, **108**, 749986, (*synth*)
Terao, S., *Adv. Prostaglandin, Thromboxane, Leukotriene Res.*, 1989, **19**, 651, (*synth, sar*)
Shiraishi, M. *et al.*, *J. Med. Chem.*, 1989, **32**, 2214, (*synth, cryst struct, pharmacol*)
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Kurokawa, T., *Biol. Pharm. Bull.*, 1994, **17**, 383, (*pharmacol*)
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