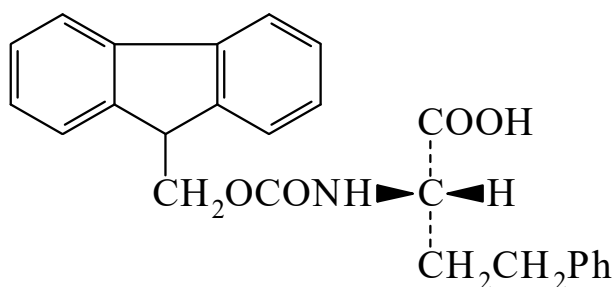




>>Entry Name: α -[[*(9H*-Fluoren-9-ylmethoxy)carbonyl]amino]benzenebutanoic acid, 9Cl

Synonym(s): NPC 14686



Molecular Formula: C₂₅H₂₃NO₄

Molecular Weight: 401.461

Accurate Mass: 401.162709

Percentage Composition: C 74.80%; H 5.77%; N 3.49%; O 15.94%

Use/Importance: Antiinflammatory agent

Calculated Log P Data: Log P 5.23 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 135944-09-1

Molecular Formula: C₂₅H₂₃NO₄

Molecular Weight: 401.461

Accurate Mass: 401.162709

Percentage Composition: C 74.80%; H 5.77%; N 3.49%; O 15.94%

Melting Point: Mp 125°

Optical Rotation: [α]_D²⁵+5.8 (c, 1 in MeOH)

>>Variant: (*S*)-form

CAS Registry Number: 132684-59-4

Molecular Formula: C₂₅H₂₃NO₄

Molecular Weight: 401.461

Accurate Mass: 401.162709

Percentage Composition: C 74.80%; H 5.77%; N 3.49%; O 15.94%

Melting Point: Mp 131°

Optical Rotation: [α]_D²⁵-6.3 (c, 1 in MeOH)

Other Data: Pharmacol. active isomer

Sigma: F7295

References:

Schiller, P.W. *et al.*, *J. Med. Chem.*, 1991, **34**, 3125, (*synth, pmr*)

Burch, R.M. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1991, **88**, 355, (*pharmacol*)