



>>Entry Name: Glycylglycylglycine

Synonym(s): Diglycylglycine. Triglycine

CAS Registry Number: 556-33-2

$\text{H}_2\text{NCH}_2\text{CONHCH}_2\text{CONHCH}_2\text{COOH}$

Molecular Formula: $\text{C}_6\text{H}_{11}\text{N}_3\text{O}_4$

Molecular Weight: 189.171

Accurate Mass: 189.074957

Percentage Composition: C 38.10%; H 5.86%; N 22.21%; O 33.83%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 246 dec.°

pKa Value: $\text{p}K_{\text{a}1}$ 3.27; $\text{p}K_{\text{a}2}$ 7.9 (25°, 0.1M KNO₃)

Fluka: 50240

Rare Chemicals Library: S44057-4

Sigma: G1377

>>Derivative: Me ester

Molecular Formula: $\text{C}_7\text{H}_{13}\text{N}_3\text{O}_4$

Molecular Weight: 203.197

Accurate Mass: 203.090607

Percentage Composition: C 41.38%; H 6.45%; N 20.68%; O 31.50%

Physical Description: Needles or prisms (CHCl₃/Et₂O)

Melting Point: Mp 111°

>>Derivative: Me ester; hydrochloride

Physical Description: Leaflets (MeOH)

Melting Point: Mp 204 dec.°

>>Derivative: Me ester; hydrobromide

Melting Point: Mp 205-207°

>>Derivative: Et ester

Molecular Formula: $\text{C}_8\text{H}_{15}\text{N}_3\text{O}_4$

Molecular Weight: 217.224

Accurate Mass: 217.106257

Percentage Composition: C 44.23%; H 6.96%; N 19.34%; O 29.46%

Physical Description: Plates (EtOH) (as hydrochloride)

Melting Point: Mp 214-219° (hydrochloride)

>>Derivative: 3,5-Dinitrobenzoyl

Physical Description: Needles (H₂O)

Melting Point: Mp 236 dec.°

>>Derivative: N-Benzyloxycarbonyl, Me ester

Melting Point: Mp 158°

References:

- Weygand, F. *et al.*, *Chem. Ber.*, 1957, **90**, 639, (*synth*)
Elias, H.G. *et al.*, *Makromol. Chem.*, 1967, **102**, 161, (*synth*)
Nekrasova, V.A. *et al.*, *Zh. Obshch. Khim.*, 1968, **37**, 1761; *CA*, **68**, 78604y, (*synth*)
Fowden, L. *et al.*, *Phytochemistry*, 1969, **8**, 1043, (*isol*)
Nagai, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 1323, (*nmr*)
Feairheller, W.R. Jr. *et al.*, *Appl. Spectrosc.*, 1971, **25**, 176, (*ir*)
Handelsman-Benory, E. *et al.*, *Acta Cryst. C*, 1995, **51**, 2362, (*cryst struct, Me ester*)