



Melting Point: Mp 231.5° (225-226°)
Optical Rotation: $[\alpha]_D +30$ (1M HCl)
Solubility: BERDY SOL: Sol. H₂O; fairly sol. MeOH
UV: [neutral] $\lambda_{\max}$ 246 () (H₂O) (Berdy) [acid] $\lambda_{\max}$ 246 () (HCl) (Berdy) [base] $\lambda_{\max}$ 260 () (NaOH) (Berdy)
Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 5000 mg/kg

>>**Derivative:** *N*⁵-(4-Methoxybenzyl)
Synonym(s): *N*⁵-(4-Methoxybenzyl)glutamine

Molecular Formula: C₁₃H₁₈N₂O₄
Molecular Weight: 266.296
Accurate Mass: 266.126658
Percentage Composition: C 58.64%; H 6.81%; N 10.52%; O 24.03%
Biological Source: Constit. of the xylem sap of the roots of *Cucurbita maxima* x *Cucurbita moschata*
Physical Description: Amorph. solid
Melting Point: Mp 214-215 dec.°
Optical Rotation: $[\alpha]_D^{22} +23$ (c, 0.1 in 1M HCl)
UV: [neutral] $\lambda_{\max}$ 224 (log ε 4.1); 273 (log ε 3.2) (H₂O)

>>**Variant:** (±)-form

CAS Registry Number: 585-21-7
Molecular Formula: C₅H₁₀N₂O₃
Molecular Weight: 146.146
Accurate Mass: 146.069143
Percentage Composition: C 41.09%; H 6.90%; N 19.17%; O 32.84%
Physical Description: Prisms (Me₂CO aq.)
Melting Point: Mp 186 dec.°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 782D, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1278B, (*nmr*)
Archibald, R.M., *Chem. Rev.*, 1945, **37**, 161, (*rev, props*)
Lepp, A. *et al.*, *Biochem. Prep.*, 1957, **5**, 79, (*synth*)
Jadot, J. *et al.*, *Biochim. Biophys. Acta*, 1960, **43**, 322, (*deriv*)
Greenstein, J.P. *et al.*, *Chemistry of the Amino Acids*, (Chapter 25), Wiley, N.Y., 1961, 1929, (*isol, synth*)
Kline, G.B. *et al.*, *J.O.C.*, 1961, **26**, 1854, (*synth*)
Larsen, P.O., *Acta Chem. Scand.*, 1965, **19**, 1071, (*N*⁵-Isopropylglutamine)
Bak, B. *et al.*, *J. Mol. Spectrosc.*, 1968, **26**, 78, (*pmr*)
Weaver, R.F. *et al.*, *J. Biol. Chem.*, 1971, **246**, 2010, (*γ*-Glutaminy-4-hydroxybenzene)
Koetzle, T.F. *et al.*, *Acta Cryst. B*, 1973, **29**, 2571, (*cryst struct*)
Voelter, W. *et al.*, *Monatsh. Chem.*, 1974, **105**, 1110, (*cmr*)
Synth. Prod. Util. Amino Acids, (Kaneko, T. *et al.*, Ed.), Halsted Press, 1974, 109, (*synth*)
Lindberg, P. *et al.*, *J.C.S. Perkin I*, 1977, 684
London, R.E. *et al.*, *J.A.C.S.*, 1978, **100**, 3723, (*cmr*)
Jaeger, P. *et al.*, *N. Engl. J. Med.*, 1986, **315**, 1120, (*rev*)
Tachiki, T. *et al.*, *Prog. Ind. Microbiol.*, 1986, **24**, 121, (*rev, synth*)
Yoshifuji, S. *et al.*, *Chem. Pharm. Bull.*, 1987, **35**, 2994, (*synth*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 328
Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, GFO050
Galinski, E.A. *et al.*, *Eur. J. Biochem.*, 1991, **198**, 593, (*N*-Carbamoylglutamineamide)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 598
Suresh, S. *et al.*, *Acta Cryst. C*, 1996, **52**, 1313, (*cryst struct, DL-form*)
Alborn, H.T. *et al.*, *Science (Washington, D.C.)*, 1997, **276**, 945-949, (*isol, Volicitin*)
Pohnert, G. *et al.*, *Chem. Comm.*, 1999, 1087-1088, (*synth, Volicitin*)
Inouye, Y. *et al.*, *Phytochemistry*, 1999, **51**, 425-428, (*N*⁵-4-Methoxybenzylglutamine)
Pohnert, G. *et al.*, *Tetrahedron*, 1999, **55**, 11275-11280, (*caterpillar amides*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, GFO050