



**Melting Point:** Mp 231.5° (225-226°)

**Optical Rotation:**  $[\alpha]_D +30$  (1M HCl)

**Solubility:** BERDY SOL: Sol. H<sub>2</sub>O; fairly sol. MeOH

**UV:** [neutral]  $\lambda_{\max}$  246 () (H<sub>2</sub>O) (Berdy) [acid]  $\lambda_{\max}$  246 () (HCl) (Berdy) [base]  $\lambda_{\max}$  260 () (NaOH) (Berdy)

**Hazard & Toxicity:** BERDY HAZD : LD<sub>50</sub> (mus, ipr) 5000 mg/kg

>>**Derivative:** *N*<sup>5</sup>-(4-Methoxybenzyl)

**Synonym(s):** *N*<sup>5</sup>-(4-Methoxybenzyl)glutamine

**Molecular Formula:** C<sub>13</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>

**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  $\epsilon$  4.1); 273 (log  $\epsilon$  3.2) (H<sub>2</sub>O)

>>**Variant:** (±)-form

**CAS Registry Number:** 585-21-7

**Molecular Formula:** C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>

**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 (Me<sub>2</sub>CO 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*<sup>5</sup>-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*<sup>5</sup>-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