



>>Entry Name: Epothilone B

CAS Registry Number: 152044-54-7

Type of Compound Code(s): VX6935 VC0100

As Epothilone A, [CGO62-V](#) with
R = CH₃

Molecular Formula: C₂₇H₄₁NO₆S

Molecular Weight: 507.69

Accurate Mass: 507.265459

Percentage Composition: C 63.88%; H 8.14%; N 2.76%; O 18.91%; S 6.32%

Biological Source: Prod. by *Sorangium cellulosum*

Biological Use/Importance: Antifungal and cytotoxic agent. Induces cellular microtubuli assembly and stabilisation by a Taxol™-like mechanism. Competes for the same binding site on microtubules as Taxol™. Antiproliferative and potential anticancer agent

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 93-94°

Optical Rotation: $[\alpha]_{\text{D}}^{21} -35$ (c, 0.7 in MeOH)

UV: [neutral] λ_{max} 211 (ϵ 18600); 249 (ϵ 14100) (MeOH)

Other Data: More potent in some cytotoxicity and antifungal assays than Epothilone A [CGO62-V](#)

References:

- Bollag, D.M., *Cancer Res.*, 1995, **55**, 2325-2333, (*pharmacol*)
Hoefle, G. *et al.*, *Angew. Chem., Int. Ed.*, 1996, **35**, 1567-1569, (*uv, pmr, cmr, cryst struct*)
Gerth, K. *et al.*, *J. Antibiot.*, 1996, **49**, 560-563, (*isol*)
Wessjohann, L. *et al.*, *Angew. Chem., Int. Ed.*, 1997, **36**, 715-718, (*rev*)
Su, D.-S. *et al.*, *Angew. Chem., Int. Ed.*, 1997, **36**, 757-759, (*synth*)
Muehlradt, P.F. *et al.*, *Cancer Res.*, 1997, **57**, 3344-3346, (*pharmacol*)
Finlay, R. *et al.*, *Chem. Ind. (London)*, 1997, 991-996, (*rev*)
Kowalski, R.J. *et al.*, *J. Biol. Chem.*, 1997, **272**, 2534-2541, (*pharmacol*)
Nicolaou, K. C. *et al.*, *J.A.C.S.*, 1997, **119**, 7960-7973; 7974-7991, (*synth*)
Meng, D. *et al.*, *J.A.C.S.*, 1997, **119**, 10073-10092, (*synth*)
Nicolaou, K.C. *et al.*, *Nature (London)*, 1997, **387**, 268-272, (*synth, bibl*)
May, S.A. *et al.*, *Chem. Comm.*, 1998, 1597-1598, (*synth*)
Mulzer, J. *et al.*, *Tet. Lett.*, 1998, **39**, 8633-8636, (*synth*)
Schinzer, D. *et al.*, *Chem. Eur. J.*, 1999, **5**, 2483-2491; 2492-2500, (*synth*)
White, J.D. *et al.*, *J.O.C.*, 1999, **64**, 684-685, (*synth, bibl*)
Taylor, R.E. *et al.*, *J.O.C.*, 1999, **64**, 7224-7228, (*conformn*)
White, J.D. *et al.*, *Org. Lett.*, 1999, **1**, 1431-1434, (*synth*)
Gerth, K. *et al.*, *J. Antibiot.*, 2000, **53**, 1373-1377, (*biosynth*)
Mulzer, J. *et al.*, *J.O.C.*, 2000, **65**, 7456-7467, (*synth*)
Mulzer, J., *Monatsh. Chem.*, 2000, **131**, 205-238, (*rev, synth*)