



>>Entry Name: Dichlorobis( $\eta^5$ -2,4-cyclopentadien-1-yl)vanadium, 9Cl  
Synonym(s): Bis(cyclopentadienyl)dichlorovanadium. Vanadocene dichloride

CAS Registry Number: 12083-48-6

As Dibromobis( $\eta^5$ -2,4-cyclopentadien-1-yl)vanadium, BQG75-U with  
X = Y = Cl

**Molecular Formula:** C<sub>10</sub>H<sub>10</sub>Cl<sub>2</sub>V

**Molecular Weight:** 252.036

**Accurate Mass:** 250.959916

**Percentage Composition:** C 47.66%; H 4.00%; Cl 28.13%; V 20.21%

**Source/Synthesis:** Synth. from VCl<sub>4</sub> and NaCp, LiCp or CpMgCl

**Use/Importance:** Co-catalyst in redn. of CO → CH<sub>4</sub>. Co-catalyst with Et<sub>2</sub>AlCl for alkene polym.; with Et<sub>3</sub>Al<sub>2</sub>Cl<sub>3</sub> for butadiene polym., with SnCl<sub>2</sub> or ZnCl<sub>2</sub> and AIBN for butadiene/acrylonitrile copolym.; and with BuLi or PhMgBr for hydrogenation of dienes to alkenes, isoprene to 2-methyl-2-butene

**Physical Description:** Dark green cryst. (CHCl<sub>3</sub>)

**Melting Point:** Mp 205 dec.°

**Solubility:** Sol. CHCl<sub>3</sub>, H<sub>2</sub>O, alcohols

**Other Data:** Dec. at 250°. Paramagnetic.  $\mu_{\text{eff}}$  = 1.71  $\mu_{\text{B}}$  (298K)

Aldrich: 33464-2

#### References:

- Wilkinson, G. *et al.*, *J.A.C.S.*, 1954, **76**, 4281, (*synth, ir*)  
*Organomet. Synth.*, 1965, **1**, 75, (*synth*)  
Tajima, Y. *et al.*, *J.O.C.*, 1968, **33**, 1689, (*use*)  
*Japan. Pat.*, 1971, 71 20 494; *CA*, **75**, 141 755k, (*use*)  
Kawasaki, A. *et al.*, *CA*, 1974, **80**, 27706, (*use*)  
Holloway, J.D.L. *et al.*, *J.A.C.S.*, 1979, **101**, 2038  
Evans, A.G. *et al.*, *J.A.C.S.*, 1979, **101**, 3204, (*use*)  
Strelets, V.V. *et al.*, *Kinet. Katal.*, 1984, **25**, 821, (*use*)  
Kopf-Maier, P. *et al.*, *Toxicology*, 1986, **38**, 81, (*tox*)  
Tzavellas, N. *et al.*, *Z. Anorg. Allg. Chem.*, 1996, **622**, 898, (*synth, cryst struct*)