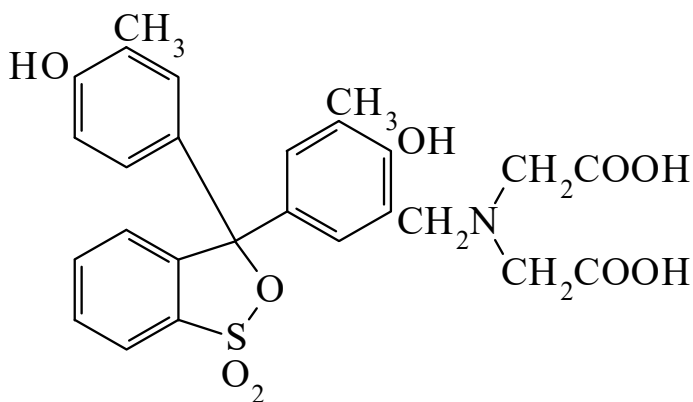




>>Entry Name: Semixylenol orange

Synonym(s): *N*-(Carboxymethyl)-*N*-[[2-hydroxy-5-[3-(4-hydroxy-3-methylphenyl)-3*H*-2,1-benzoxathiol-3-yl]-3-methylphenyl]methyl]glycine *S,S*-dioxide, 9Cl



CAS Registry Number: 19329-67-0

Molecular Formula: C₂₆H₂₅NO₉S

Molecular Weight: 527.551

Accurate Mass: 527.125004

Percentage Composition: C 59.20%; H 4.78%; N 2.66%; O 27.29%; S 6.08%

Use/Importance: Used as EtOH soln. for photometric detn. of Zr (λ_{max} 533nm, ϵ 59000)

Physical Description: Red cryst. powder

Solubility: Sol. H₂O, alkalis; sl. sol. EtOH

pKa Value: p*K*_{a5} 2.6; p*K*_{a7} 7.47; p*K*_{a8} 10.9 (25°, μ = 1)

References:

Olson, D.C. *et al.*, *Anal. Chem.*, 1962, **34**, 1299, (*detn*, Zr)

Murakami, M. *et al.*, *Talanta*, 1967, **14**, 1293, (*synth*)