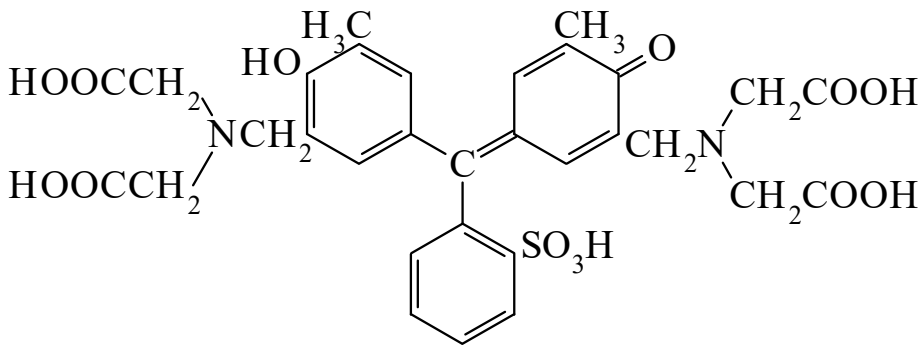
>>**Entry Name: Xylenol orange**

Synonym(s): *N*,*N*'-[3*H*-2,1-Benzoxathiol-3-ylidenebis[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]bis[*N*-(carboxymethyl)glycine] *S*,*S*-dioxide, 9Cl. 3,3'-Bis[*N*,*N*-di(carboxymethyl)aminomethyl]-*o*-cresolsulfonephthalein. *o*-Cresolphthalexone S



CAS Registry Number: 1611-35-4
Related CAS Registry Numbers(s): 3618-43-7

Molecular Formula: $C_{31}H_{32}N_2O_{13}S$
Molecular Weight: 672.665
Accurate Mass: 672.162513
Percentage Composition: C 55.35%; H 4.79%; N 4.16%; O 30.92%; S 4.77%
Use/Importance: Used as 0.05% aq. soln. for spectrophotometric detn. of Bi (λ_{max} 545 nm, ε 24000), Zr (λ_{max} 535 nm, ε 35000), Hg, Nb, Sc, Y, Zn, Al, Th, Ga, U, V; as an indicator in EDTA titrations. Mono- and tetrasodium salts are also used
Physical Description: Dark red cryst. powder
Melting Point: Mp 286 dec.°
Solubility: Sol. H_2O
pKa Value: pK_{a5} 2.58; pK_{a7} 6.4; pK_{a8} 10.5 (25°)

>>**Derivative:** Mono-Na salt

CAS Registry Number: 63721-83-5
Physical Description: Dark red cryst. powder
Melting Point: Mp 210 dec.°
Other Data: λ_{max} 580 nm
Fluka: 95615

References:

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Cabrera-Martin, A. *et al.*, *Talanta*, 1969, **16**, 1023, *(detn, Hg)*
Leong, C.L.*, Anal. Chem.*, 1973, **45**, 21, *(detn, U)*
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