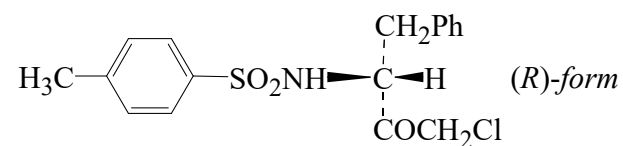




>>Entry Name: *N*-[3-Chloro-2-oxo-1-(phenylmethyl)propyl]-4-methylbenzenesulfonamide, 9Cl

Synonym(s): *N*-[α -(Chloroacetyl)phenethyl]-*p*-toluenesulfonamide, 8Cl. TPCK



CAS Registry Number: 329-30-6

Molecular Formula: $\text{C}_{17}\text{H}_{18}\text{ClNO}_3\text{S}$

Molecular Weight: 351.853

Accurate Mass: 351.069591

Percentage Composition: C 58.03%; H 5.16%; Cl 10.08%; N 3.98%; O 13.64%; S 9.11%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 18945-32-9

Molecular Formula: $\text{C}_{17}\text{H}_{18}\text{ClNO}_3\text{S}$

Molecular Weight: 351.853

Accurate Mass: 351.069591

Percentage Composition: C 58.03%; H 5.16%; Cl 10.08%; N 3.98%; O 13.64%; S 9.11%

Melting Point: Mp 103-104°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -10.1$ (c, 3.56 in CHCl_3)

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 402-71-1

Molecular Formula: $\text{C}_{17}\text{H}_{18}\text{ClNO}_3\text{S}$

Molecular Weight: 351.853

Accurate Mass: 351.069591

Percentage Composition: C 58.03%; H 5.16%; Cl 10.08%; N 3.98%; O 13.64%; S 9.11%

Use/Importance: Inhibitor of chymotrypsin, papain and *E. coli* proteases. Inactive against trypsin

Melting Point: Mp 103-104°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -88$ (c, 1 in EtOH). $[\alpha]_{\text{D}}^{25} +9.7$ (c, 5 in CHCl_3)

References:

Schoellman, G. *et al.*, *Biochemistry*, 1963, **2**, 252-255, (*S*-form, synth, biochem)

Bender, M.L. *et al.*, *J.A.C.S.*, 1966, **88**, 5880-5889, (*biochem*)

Michel, A. *et al.*, *Bull. Soc. Chim. Belg.*, 1980, **89**, 25-32, (*cryst, struct*)