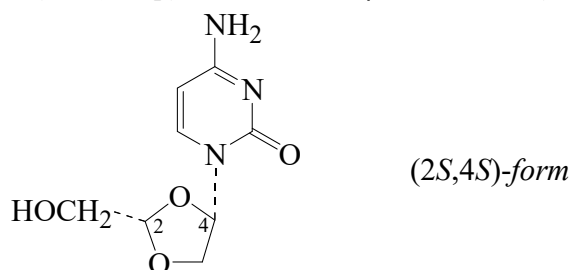




>>Entry Name: Troxacitabine, INN, USAN

Synonym(s): 4-Amino-1-[2-(hydroxymethyl)-1,3-dioxolan-4-yl]-2(1*H*)-pyrimidinone, 9Cl. β -L-Dioxolanecytidine. BCH 4556



Related CAS Registry Numbers(s): 126652-17-3 145511-98-4 151282-98-3

Molecular Formula: C₈H₁₁N₃O₄

Molecular Weight: 213.193

Accurate Mass: 213.074957

Percentage Composition: C 45.07%; H 5.20%; N 19.71%; O 30.02%

Biological Use/Importance: Antineoplastic agent. Anti-HIV agent

Other Data: The name troxacitabine refers to the (2*S*,4*S*)-form

>>Variant: (2*R*,4*R*)-form

CAS Registry Number: 141196-84-1

Molecular Formula: C₈H₁₁N₃O₄

Molecular Weight: 213.193

Accurate Mass: 213.074957

Percentage Composition: C 45.07%; H 5.20%; N 19.71%; O 30.02%

Melting Point: Mp 181-183°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +35.2$ (c, 1.0 in MeOH)

>>Variant: (2*R*,4*S*)-form

Synonym(s): (-)-BCH 203

CAS Registry Number: 141196-85-2

Molecular Formula: C₈H₁₁N₃O₄

Molecular Weight: 213.193

Accurate Mass: 213.074957

Percentage Composition: C 45.07%; H 5.20%; N 19.71%; O 30.02%

Melting Point: Mp 188-190°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -68.5$ (c, 0.5 in MeOH)

>>Variant: (2*S*,4*R*)-form

CAS Registry Number: 145416-37-1

Molecular Formula: C₈H₁₁N₃O₄

Molecular Weight: 213.193

Accurate Mass: 213.074957

Percentage Composition: C 45.07%; H 5.20%; N 19.71%; O 30.02%

Physical Description: Cryst. (CH₂Cl₂/hexane)

Melting Point: Mp 192-193°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +66.14$ (c, 0.5 in MeOH)

UV: [neutral] λ_{max} 278 (ϵ 13240) (pH2) [neutral] λ_{max} 270 (ϵ 8780) (pH7) [neutral] λ_{max} 269 (ϵ 9070) (pH11)

>>Variant: (2*S*,4*S*)-form

Synonym(s): (-)-BCH 204

CAS Registry Number: 145918-75-8

Molecular Formula: C₈H₁₁N₃O₄

Molecular Weight: 213.193

Accurate Mass: 213.074957

Percentage Composition: C 45.07%; H 5.20%; N 19.71%; O 30.02%

Physical Description: Cryst. (CH₂Cl₂/hexane)

Melting Point: Mp 176-177°

Optical Rotation: $[\alpha]_{\text{D}}^{24} -38.33$ (c, 0.43 in MeOH)

UV: [neutral] λ_{max} 278 (ϵ 11970) (pH2) [neutral] λ_{max} 270 (ϵ 7770) (pH7) [neutral] λ_{max} 269 (ϵ 8380) (pH11)

References: