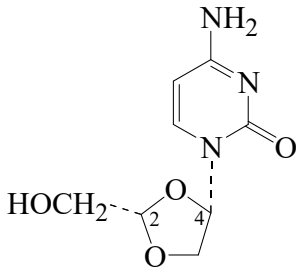
>>**Entry Name: Troxacitabine,** INN, USAN

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



(2*S*,4*S*)-*form*

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

Molecular Formula: $C_8H_{11}N_3O_4$
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: $C_8H_{11}N_3O_4$
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: $[\alpha]_D^{22}$+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: $C_8H_{11}N_3O_4$
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: $[\alpha]_D^{22}$–68.5 (c, 0.5 in MeOH)

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

CAS Registry Number: 145416-37-1
Molecular Formula: $C_8H_{11}N_3O_4$
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. (CH_2Cl_2/hexane)
Melting Point: Mp 192-193°
Optical Rotation: $[\alpha]_D^{25}$+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: $C_8H_{11}N_3O_4$
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. (CH_2Cl_2/hexane)
Melting Point: Mp 176-177°
Optical Rotation: $[\alpha]_D^{24}$–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: