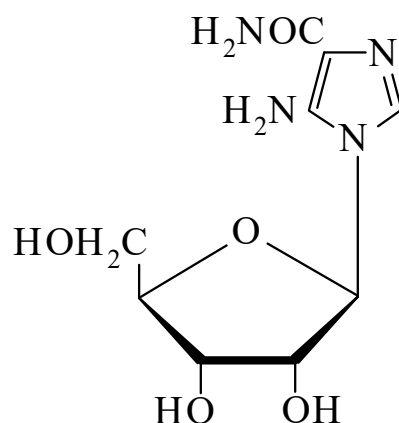




>>Entry Name: Acadesine, BAN, INN, USAN

ENTRY UNDER REVIEW

Synonym(s): 5-Amino-1-ribofuranosyl-1*H*-imidazole-4-carboxamide, 9Cl. AICA-Riboside. AICAR. GP 1-110



CAS Registry Number: 2627-69-2

Molecular Formula: C<sub>9</sub>H<sub>14</sub>N<sub>4</sub>O<sub>5</sub>

Molecular Weight: 258.233

Accurate Mass: 258.096421

Percentage Composition: C 41.86%; H 5.46%; N 21.70%; O 30.98%

Source/Synthesis: Accumulates in the culture medium of *E. coli* under sulfonamide stasis. Manuf. by *Bacillus pumilus* and *Bacillus subtilis*

Use/Importance: Platelet aggregation inhibitor

Physical Description: Pink rosettes (EtOH)

Melting Point: Mp 215-216 dec.°

Optical Rotation:  $[\alpha]_D^{27} -62.4$  (c, 0.5 in H<sub>2</sub>O)

Solubility: BERDY SOL: Sol. H<sub>2</sub>O

Calculated Log P Data: Log P -2.97 (calc)

Sigma: A8129

>>Derivative: Picrate

CAS Registry Number: 24418-25-5

Melting Point: Mp 146-147°

>>Derivative: 2',3',5'-Tri-Ac

CAS Registry Number: 23274-21-7

Molecular Formula: C<sub>15</sub>H<sub>20</sub>N<sub>4</sub>O<sub>8</sub>

Molecular Weight: 384.345

Accurate Mass: 384.128116

Percentage Composition: C 46.88%; H 5.24%; N 14.58%; O 33.30%

Melting Point: Mp 69° (88-90°, 130-131°)

Optical Rotation:  $[\alpha]_D^{27} -30.5$  (c, 1.0 in EtOH)

>>Derivative: N,2',3',5'-Tetra-Ac

CAS Registry Number: 37805-74-6

Molecular Formula: C<sub>17</sub>H<sub>22</sub>N<sub>4</sub>O<sub>9</sub>

Molecular Weight: 426.382

Accurate Mass: 426.138681

Percentage Composition: C 47.89%; H 5.20%; N 13.14%; O 33.77%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 208-209°

Optical Rotation:  $[\alpha]_D^{26} +2.9$  (c, 0.51 in CHCl<sub>3</sub>)

>>Derivative: 2',3'-O-Isopropylidene, 5'-Ac

Molecular Formula: C<sub>14</sub>H<sub>20</sub>N<sub>4</sub>O<sub>6</sub>

Molecular Weight: 340.335

Accurate Mass: 340.138286

Percentage Composition: C 49.41%; H 5.92%; N 16.46%; O 28.21%

Melting Point: Mp 168-169°