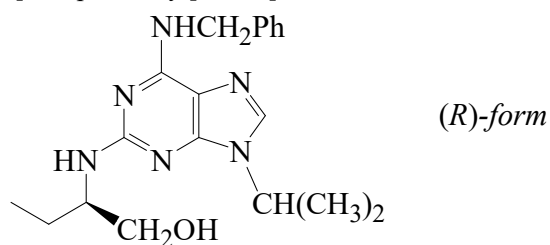




>>Entry Name: Roscovitine

Synonym(s): 2-[[9-(1-Methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-1-butanol, 9Cl



CAS Registry Number: 186692-44-4

Molecular Formula: C<sub>19</sub>H<sub>26</sub>N<sub>6</sub>O

Molecular Weight: 354.454

Accurate Mass: 354.216809

Percentage Composition: C 64.38%; H 7.39%; N 23.71%; O 4.51%

Biological Use/Importance: Cyclin-dependent kinase inhibitor. Antineoplastic agent. Cytokinin

>>Variant: (R)-form

CAS Registry Number: 186692-46-6

Molecular Formula: C<sub>19</sub>H<sub>26</sub>N<sub>6</sub>O

Molecular Weight: 354.454

Accurate Mass: 354.216809

Percentage Composition: C 64.38%; H 7.39%; N 23.71%; O 4.51%

Melting Point: Mp 102-104°

Optical Rotation:  $[\alpha]_D^{20} -34.6$  (c, 0.43 in CHCl<sub>3</sub>)

Other Data: Pharmacol. active isomer

>>Variant: (S)-form

CAS Registry Number: 186692-45-5

Molecular Formula: C<sub>19</sub>H<sub>26</sub>N<sub>6</sub>O

Molecular Weight: 354.454

Accurate Mass: 354.216809

Percentage Composition: C 64.38%; H 7.39%; N 23.71%; O 4.51%

Melting Point: Mp 118-120°

Optical Rotation:  $[\alpha]_D^{20} +35.3$  (c, 0.57 in CHCl<sub>3</sub>)

>>Variant: (±)-form

Molecular Formula: C<sub>19</sub>H<sub>26</sub>N<sub>6</sub>O

Molecular Weight: 354.454

Accurate Mass: 354.216809

Percentage Composition: C 64.38%; H 7.39%; N 23.71%; O 4.51%

Physical Description: Cryst. (CHCl<sub>3</sub>/Et<sub>2</sub>O)

Melting Point: Mp 137-139°

References:

Pippin, J.W. *et al.*, *J. Clin. Invest.*, 1997, **100**, 2512-2520, (*pharmacol*)

Havlicek, L. *et al.*, *J. Med. Chem.*, 1997, **40**, 408-412, (*synth, pharmacol*)

*Pat. Coop. Treaty (WIPO)*, 1997, CNRS, 97 20 842; *CA*, **127**, 104333t, (*synth, pharmacol*)

Mgbonyebi, O.P. *et al.*, *Cancer Res.*, 1999, **59**, 1903-1910, (*pharmacol*)