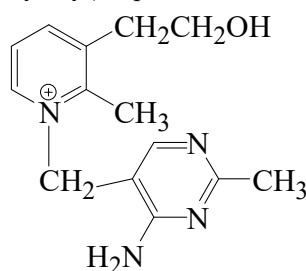




>>Entry Name: 1-[(4-Amino-2-methyl-5-pyrimidinyl)methyl]-3-(2-hydroxyethyl)-2-methylpyridinium(1+), 9Cl

Synonym(s): 1-[(4-Amino-2-methyl-5-pyrimidinyl)methyl]-3-(2-hydroxyethyl)-2-picolinium, 8Cl. Pyrithiamine. Neopyrithiamine (obsol.)



CAS Registry Number: 5593-78-2

Molecular Formula: C₁₄H₁₉N₄O⁽⁺⁾

Molecular Weight: 259.33

Accurate Mass: 259.155886

Percentage Composition: C 64.84%; H 7.38%; N 21.60%; O 6.17%

Use/Importance: Thiamine antagonist

Other Data: Strictly the trade names refer to the bromide

>>Derivative: Chloride

CAS Registry Number: 554-33-6

Molecular Formula: C₁₄H₁₉ClN₄O

Molecular Weight: 294.783

Accurate Mass: 294.124738

Percentage Composition: C 57.04%; H 6.50%; Cl 12.03%; N 19.01%; O 5.43%

Melting Point: Mp 234-236° (dec.) (as hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: Bromide

CAS Registry Number: 534-64-5

Molecular Formula: C₁₄H₁₉BrN₄O

Molecular Weight: 339.234

Accurate Mass: 338.094222

Percentage Composition: C 49.57%; H 5.65%; Br 23.55%; N 16.52%; O 4.72%

Physical Description: Cryst. (Me₂CO) (as hydrobromide)

Melting Point: Mp 205-210° (hydrobromide). Mp 218-220° (dec.) (hydrobromide)

Other Data: CAS no. refers to hydrobromide

References:

Tracy, A.H. *et al.*, *J.O.C.*, 1941, **6**, 54-62, (*synth*)

Wilson, A.N. *et al.*, *J.A.C.S.*, 1949, **71**, 2231-2233, (*synth*)

Woodley, D.W., *J.A.C.S.*, 1950, **72**, 5763-5765, (*props, nomencl*)

Gallo, A.A. *et al.*, *J. Biol. Chem.*, 1974, **249**, 1382-1382, (*cmr*)

Shin, W. *et al.*, *J.A.C.S.*, 1993, **115**, 12238-12250, (*conformn*)

Merck Index, 12th edn., 1996, 8176, (*bibl, props*)