



>>Entry Name: *N,N'*-Bis(2-chloroethyl)phosphorodiamidic acid

Synonym(s): Isophosphoramidate mustard

CAS Registry Number: 31645-39-3

$(\text{ClCH}_2\text{CH}_2\text{NH})_2\text{P}(\text{O})\text{OH}$

Molecular Formula: $\text{C}_4\text{H}_{11}\text{Cl}_2\text{N}_2\text{O}_2\text{P}$

Molecular Weight: 221.022

Accurate Mass: 219.993519

Percentage Composition: C 21.74%; H 5.02%; Cl 32.08%; N 12.67%; O 14.48%; P 14.01%

Use/Importance: Active metab. of Ifosfamide [GGL76-F](#) and as active as Cyclophosphamide [CZG78-T](#) against leukomas and carcinomas

Physical Description: Cryst.

Melting Point: Mp 106-107°. Mp 137-138°

>>Derivative: 3-Butenyl ester

Synonym(s): 3-Butenyl *N,N'*-bis(2-chloroethyl)phosphorodiamidate

Molecular Formula: $\text{C}_8\text{H}_{17}\text{Cl}_2\text{N}_2\text{O}_2\text{P}$

Molecular Weight: 275.114

Accurate Mass: 274.040469

Percentage Composition: C 34.93%; H 6.23%; Cl 25.77%; N 10.18%; O 11.63%; P 11.26%

Physical Description: Oil

References:

Takamizawa, A. *et al.*, *Chem. Pharm. Bull.*, 1977, **25**, 1877, (*ester, pmr*)

Misiura, K. *et al.*, *J. Med. Chem.*, 1983, **26**, 674, (*synth, ester, ms, P nmr*)

Struck, R.F. *et al.*, *Br. J. Cancer*, 1983, **47**, 15, (*metab, ir, pmr*)