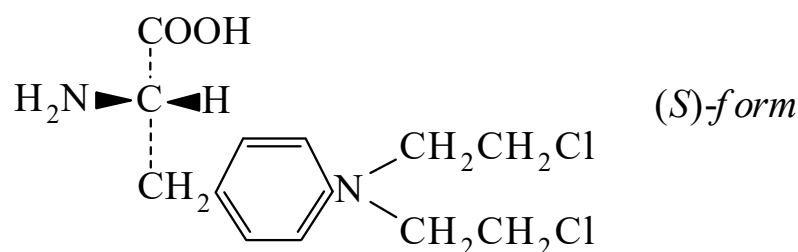




>>Entry Name: **Melphalan**, BAN, INN, JAN, USAN

Synonym(s): 4-[Bis(2-chloroethyl)amino]phenylalanine. Alanine nitrogen mustard. Phenylalanine Lost. Phenylalanine-Mustard. Sarcolysin. **PAM**‡



Molecular Formula: C₁₃H₁₈Cl₂N₂O₂

Molecular Weight: 305.203

Accurate Mass: 304.074532

Percentage Composition: C 51.16%; H 5.94%; Cl 23.23%; N 9.18%; O 10.48%

Use/Importance: Alkylating agent used for treatment of multiple myeloma. Antineoplastic agent

Calculated Log P Data: Log P -0.34 (uncertain value) (calc)

>>Variant: (R)-form

Synonym(s): D-form. Medphalan. Medfalan. CB 3026. NSC 35051

CAS Registry Number: 13045-94-8

Molecular Formula: C₁₃H₁₈Cl₂N₂O₂

Molecular Weight: 305.203

Accurate Mass: 304.074532

Percentage Composition: C 51.16%; H 5.94%; Cl 23.23%; N 9.18%; O 10.48%

Physical Description: Needles + 1MeOH (MeOH)

Melting Point: Mp 181.5-182 dec.°

Optical Rotation: [α]_D²¹ -7.5 (c, 1.26 in M HCl)

Hazard & Toxicity: Adverse effects (bone marrow depression, gastrointestinal disturbance) reported when used therapeutically. LD₅₀ (mus, ivn) 1200 mg/kg

>>Variant: (S)-form

Synonym(s): L-form. Melfalan. Alkeran. CB 3025. NSC 8806. SK 15673

CAS Registry Number: 148-82-3

Molecular Formula: C₁₃H₁₈Cl₂N₂O₂

Molecular Weight: 305.203

Accurate Mass: 304.074532

Percentage Composition: C 51.16%; H 5.94%; Cl 23.23%; N 9.18%; O 10.48%

Physical Description: Needles + 1MeOH (MeOH)

Melting Point: Mp 182-183 dec.°

Optical Rotation: [α]_D²² +7.5 (c, 1.33 in 1M HCl). [α]_D -31.5 (c, 0.67 in MeOH)

Hazard & Toxicity: Human carcinogen. Adverse effects reported when used therapeutically or from occup. exposure. Skin irritant. LD₅₀ (rat, orl) 11 mg/kg. Human reprod. effects

Fluka: 63648

Sigma: M2011

>>Variant: (±)-form

Synonym(s): Merphalen. Merfalan. Racemalfalan. Sarcoclorin. CB 3007. NSC 14210

CAS Registry Number: 531-76-0

Molecular Formula: C₁₃H₁₈Cl₂N₂O₂

Molecular Weight: 305.203

Accurate Mass: 304.074532

Percentage Composition: C 51.16%; H 5.94%; Cl 23.23%; N 9.18%; O 10.48%

Physical Description: Needles (MeOH)

Melting Point: Mp 180-181°

Hazard & Toxicity: Possible human carcinogen. LD₅₀ (rat, orl) 105 mg/kg. Exp. reprod. and teratogenic effects

>>Derivative: Hydrochloride

CAS Registry Number: 1465-26-5

Physical Description: Cryst. (EtOH)

Melting Point: Mp 182-185°