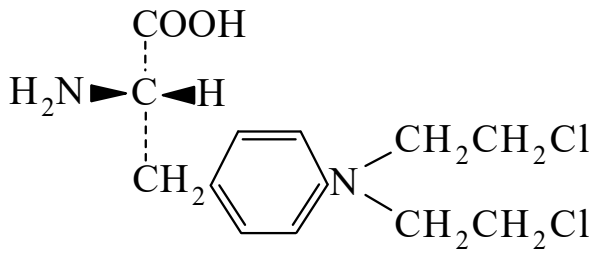
>>**Entry Name: Melphalan,** BAN, INN, JAN, USAN
Synonym(s): 4-[Bis(2-chloroethyl)amino]phenylalanine. Alanine nitrogen mustard. Phenylalanine Lost. Phenylalanine-Mustard. Sarcolysin. **PAM‡**



(*S*)-*form*

Molecular Formula: $C_{13}H_{18}Cl_2N_2O_2$
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: $C_{13}H_{18}Cl_2N_2O_2$
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: $[\alpha]_D^{21}$ –7.5 (c, 1.26 in *M* HCl)
Hazard & Toxicity: Adverse effects (bone marrow depression, gastrointestinal disturbance) reported when used therapeutically. LD_{50} (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: $C_{13}H_{18}Cl_2N_2O_2$
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: $[\alpha]_D^{22}$ +7.5 (c, 1.33 in 1*M* HCl). $[\alpha]_D$ –31.5 (c, 0.67 in MeOH)
Hazard & Toxicity: Human carcinogen. Adverse effects reported when used therapeutically or from occup. exposure. Skin irritant. LD_{50} (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: $C_{13}H_{18}Cl_2N_2O_2$
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. LD_{50} (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°

https://www.baizuoyan.com - CopyRight ©baizuoyan