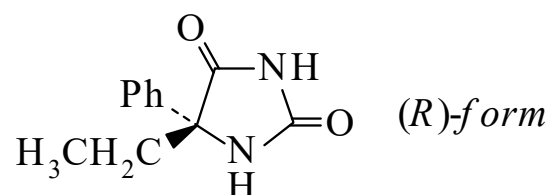




>>Entry Name: 5-Ethyl-5-phenyl-2,4-imidazolidione, 9CI
Synonym(s): 5-Ethyl-5-phenylhydantoin, 8CI. Nirvanol. AC 1050



CAS Registry Number: 631-07-2

Molecular Formula: $C_{11}H_{12}N_2O_2$
Molecular Weight: 204.228
Accurate Mass: 204.089878
Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%
Use/Importance: Anticonvulsant and hypnotic
Calculated Log P Data: Log P 1.58 (calc)
Hazard & Toxicity: Eye, skin and mucous membrane irritant

Rare Chemicals Library: S45338-2

>>Variant: (*R*)-form

CAS Registry Number: 65567-32-0
Molecular Formula: $C_{11}H_{12}N_2O_2$
Molecular Weight: 204.228
Accurate Mass: 204.089878
Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 235-237°
Optical Rotation: $[\alpha]_D -121$ (EtOH). $[\alpha]_D -167$ (alkali aq.)
Hazard & Toxicity: Adverse effects by ingestion incl. allergic dermatitis. LD₅₀ (mus, ipr) 500 mg/kg. Exp. reprod. and teratogenic effects

>>Variant: (*S*)-form

CAS Registry Number: 65567-34-2
Molecular Formula: $C_{11}H_{12}N_2O_2$
Molecular Weight: 204.228
Accurate Mass: 204.089878
Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%
Use/Importance: Slightly less effective than ($\pm$)-form, but only one-third as toxic.
Physical Description: Flaky platelets (EtOH aq.)
Melting Point: Mp 237°
Optical Rotation: $[\alpha]_D +123$ (EtOH). $[\alpha]_D +169$ (alkali aq.)

>>Variant: ($\pm$)-form

CAS Registry Number: 2216-93-5
Molecular Formula: $C_{11}H_{12}N_2O_2$
Molecular Weight: 204.228
Accurate Mass: 204.089878
Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%
Physical Description: Needles or prisms (EtOH aq.)
Melting Point: Mp 199-200°
Solubility: Spar. sol. hot H₂O; insol. C₆H₆; sol. warm EtOH
pKa Value: pK_{a1} 8.5
Other Data: Causes muscular damage

References: