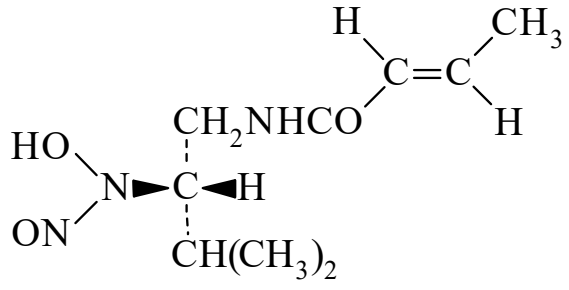
>>**Entry Name: Dopastin**
Synonym(s): *N*-[2-(Hydroxynitrosoamino)-3-methylbutyl]-2-butenamide, 9CI



Type of Compound Code(s): XA1950 XA3950 XA1650

Molecular Formula: $C_9H_{17}N_3O_3$
Molecular Weight: 215.252
Accurate Mass: 215.126992
Percentage Composition: C 50.22%; H 7.96%; N 19.52%; O 22.30%
Use/Importance: Dopamine β-hydroxylase inhibitor. Antihypertensive, antineoplastic agent
Solubility: BERDY SOL: Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O
UV: [acid] λ_{max} 215 (ε 20900) (0.01*N* HCl) (Derep) [base] λ_{max} 213 (ε 17800); 246 (ε 10800) (0.01*N* NaOH) (Derep) [neutral] λ_{max} 213 (ε 18100); 245 (ε 10500) (pH 7 phosphate buffer) (Derep) [neutral] λ_{max} 213 (E1%/1cm 840); 245 (E1%/1cm 190) (pH 7 buffer) (Berdy) [acid] λ_{max} 215 (E1%/1cm 970) (HCl) (Berdy) [base] λ_{max} 213 (E1%/1cm 330); 246 (E1%/1cm 500) (NAOH) (Berdy)

>>**Variant:** (*S,E*)-form

CAS Registry Number: 37134-80-8
Type of Compound Code(s): VV0130 AH0130
Molecular Formula: $C_9H_{17}N_3O_3$
Molecular Weight: 215.252
Accurate Mass: 215.126992
Percentage Composition: C 50.22%; H 7.96%; N 19.52%; O 22.30%
Biological Source: Obt. from *Pseudomonas* bacteria
Melting Point: Mp 116-119°
Optical Rotation: $[\alpha]_D^{21}$ –246 (c, 0.5 in EtOH)
pKa Value: pK_a 5.1
Other Data: Pharmacol. active isomer
Hazard & Toxicity: LD_{50} (mus, orl) 750 mg/kg. LD_{50} (mus, ipr) 460 mg/kg

References:

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Ohno, M. *et al.*, *Chem. Comm.*, 1973, 147, *(abs config)*
Umezawa, H., *Pure Appl. Chem.*, 1973, **33**, 129, *(pharmacol)*
Iinuma, H. *et al.*, *Agric. Biol. Chem.*, 1974, **38**, 2099, *(synth, props)*

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