



>>Entry Name: **2,2-Diethyl-4-pentenoic acid**, 9CI

Synonym(s): Diethylallylacetic acid

CAS Registry Number: 67020-02-4

$\text{H}_2\text{C}=\text{CHCH}_2\text{C}(\text{CH}_2\text{CH}_3)_2\text{COOH}$

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_2$

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

>>Derivative: Amide

Synonym(s): Diethylallylacetamide. **Valdetamide**, INN. Epinoval. Novonal. DAPA

CAS Registry Number: 512-48-1

Molecular Formula: $\text{C}_9\text{H}_{17}\text{NO}$

Molecular Weight: 155.239

Accurate Mass: 155.131014

Percentage Composition: C 69.63%; H 11.04%; N 9.02%; O 10.31%

Use/Importance: Mild hypnotic

Melting Point: Mp 75-76°

Calculated Log P Data: Log P 1.64 (calc)

Hazard & Toxicity: LD₅₀ (hmn, orl) 300 mg/kg. LD₅₀ (rat, orl) 400 mg/kg

References:

Bockmühl, M. *et al.*, *Dtsch. Med. Wochenschr.*, 1928, **54**, 270; 271, (*amide*)

Beyer, K.H., *Dtsch. Apoth. -Ztg.*, 1978, **118**, 1303, (*rev, amide*)

Klug, E. *et al.*, *Arzneim.-Forsch.*, 1979, **29**, 1651, (*anal, metab, amide*)

Eur. Pat., 1981, *Sterwin*, 33 233; *CA*, **95**, 203337, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DJU200