



>>Entry Name: 2-Oxopentanoic acid, 9CI  
Synonym(s): 2-Oxovaleric acid.  $\alpha$ -Ketovaleric acid

CAS Registry Number: 1821-02-9

$\text{H}_3\text{CCH}_2\text{CH}_2\text{COCOOH}$

Molecular Formula:  $\text{C}_5\text{H}_8\text{O}_3$   
Molecular Weight: 116.116  
Accurate Mass: 116.047345  
Percentage Composition: C 51.72%; H 6.94%; O 41.34%  
Biological Source: Isol. from *Trigonella caerulea*  
Physical Description: Liq.  
Melting Point: Mp 6-7°  
Boiling Point: Bp 179°. Bp<sub>12</sub> 78°  
Solubility: Mod. sol.  $\text{H}_2\text{O}$   
Density:  $d_4^{14}$  1.097  
Refractive Index:  $n_D^{20}$  1.4283

Fluka: 75950  
Sigma: K9250

>>Derivative: Na salt

CAS Registry Number: 13022-83-8  
Physical Description: Cryst.  
Melting Point: Mp 236°

>>Derivative: Oxime  
Synonym(s): 2-(Hydroxyimino)pentanoic acid, 9CI

CAS Registry Number: 21486-54-4  
Molecular Formula:  $\text{C}_5\text{H}_9\text{NO}_3$   
Molecular Weight: 131.131  
Accurate Mass: 131.058244  
Percentage Composition: C 45.80%; H 6.92%; N 10.68%; O 36.60%  
Physical Description: Needles (petrol)  
Melting Point: Mp 145°

>>Derivative: Phenylhydrazone

Physical Description: Cryst.  
Melting Point: Mp 101-102°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)  
Melting Point: Mp 220 dec.°

>>Derivative: Me ester

CAS Registry Number: 6376-59-6  
Molecular Formula:  $\text{C}_6\text{H}_{10}\text{O}_3$   
Molecular Weight: 130.143  
Accurate Mass: 130.062995  
Percentage Composition: C 55.37%; H 7.74%; O 36.88%  
Physical Description: Liq.  
Boiling Point: Bp<sub>12</sub> 60-62°

>>Derivative: Et ester

CAS Registry Number: 50461-74-0  
Molecular Formula:  $\text{C}_7\text{H}_{12}\text{O}_3$   
Molecular Weight: 144.17  
Accurate Mass: 144.078645  
Percentage Composition: C 58.32%; H 8.39%; O 33.29%  
Physical Description: Liq.  
Boiling Point: Bp 179-180°. Bp<sub>11</sub> 70.5°