



>>Entry Name: 1,2-Decanediol, 9CI

CAS Registry Number: 1119-86-4

Related CAS Registry Numbers(s): 87827-60-9

$\text{H}_3\text{C}(\text{CH}_2)_7\text{CH}(\text{OH})\text{CH}_2\text{OH}$

Molecular Formula:  $\text{C}_{10}\text{H}_{22}\text{O}_2$

Molecular Weight: 174.283

Accurate Mass: 174.16198

Percentage Composition: C 68.92%; H 12.72%; O 18.36%

Aldrich: 26032-0

>>Variant: (S)-form

CAS Registry Number: 84276-14-2

Molecular Formula:  $\text{C}_{10}\text{H}_{22}\text{O}_2$

Molecular Weight: 174.283

Accurate Mass: 174.16198

Percentage Composition: C 68.92%; H 12.72%; O 18.36%

Physical Description: Cryst. ( $\text{Et}_2\text{O}$ /hexane)

Melting Point: Mp 48-50°

Optical Rotation:  $[\alpha]_{\text{D}}^{22} -12.2$  (c, 0.586 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 81096-87-9

Molecular Formula:  $\text{C}_{10}\text{H}_{22}\text{O}_2$

Molecular Weight: 174.283

Accurate Mass: 174.16198

Percentage Composition: C 68.92%; H 12.72%; O 18.36%

Melting Point: Mp 48-49°

Boiling Point: Bp 255°

#### References:

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **1**, 206A, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 136C, (*ir*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 198D, (*ir*)

Swern, D. *et al.*, *J.A.C.S.*, 1946, **68**, 1504, (*synth*)

Sharpless, K.B. *et al.*, *J.A.C.S.*, 1976, **98**, 1986

Chattopadhyay, S. *et al.*, *Tetrahedron*, 1990, **46**, 3667, (*synth, ir, pmr*)