



>>Entry Name: **3-(4-Chlorophenyl)propenal**, 9Cl

Synonym(s): *p*-Chlorocinnamaldehyde, 8Cl

CAS Registry Number: 1075-77-0

Structure by analogy with 3-(2-Chlorophenyl)propenal, [DWQ21-L](#)

Molecular Formula: C<sub>9</sub>H<sub>7</sub>ClO

Molecular Weight: 166.606

Accurate Mass: 166.018542

Percentage Composition: C 64.88%; H 4.23%; Cl 21.28%; O 9.60%

Rare Chemicals Library: S94996-5

>>Variant: (*E*)-form

CAS Registry Number: 49678-02-6

Molecular Formula: C<sub>9</sub>H<sub>7</sub>ClO

Molecular Weight: 166.606

Accurate Mass: 166.018542

Percentage Composition: C 64.88%; H 4.23%; Cl 21.28%; O 9.60%

Physical Description: Prisms or needles

Melting Point: Mp 62-62.5°

Boiling Point: Bp<sub>14</sub> 155-156°

>>Derivative: Semicarbazone

Melting Point: Mp 231°

#### References:

- Pfister-Guillouzo, G. *et al.*, *Bull. Soc. Chim. Fr.*, 1964, 3252-3253, (*synth, ir*)  
Izawa, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 555-558, (*synth*)  
Olsen, D.K. *et al.*, *J.O.C.*, 1980, **45**, 4049-4052, (*synth, ir*)  
Unterhalt, B. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 574, (*synth*)  
Myrboh, B. *et al.*, *J.O.C.*, 1983, **48**, 5327-5332, (*synth*)  
Jeffery, T., *Chem. Comm.*, 1984, 1287-1289, (*synth*)  
Huang, Y. *et al.*, *Tet. Lett.*, 1985, **26**, 6447-6448, (*synth*)  
Frey, H., *Synlett*, 1990, 215, (*synth*)  
Kolehmainen, E. *et al.*, *Magn. Reson. Chem.*, 1991, **29**, 1109-1113, (*pmr, cmr, O-17 nmr*)