



>>Entry Name: Heptylbenzene, 9CI

Synonym(s): 1-Phenylheptane, 8CI

CAS Registry Number: 1078-71-3

Ph(CH<sub>2</sub>)<sub>6</sub>CH<sub>3</sub>

Molecular Formula: C<sub>13</sub>H<sub>20</sub>

Molecular Weight: 176.301

Accurate Mass: 176.1565

Percentage Composition: C 88.57%; H 11.43%

Physical Description: Liq.

Boiling Point: Bp 240°. Bp<sub>10</sub> 108-110°

Density: d<sub>4</sub><sup>20</sup> 0.857

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4865

Aldrich: 11318-2

Fluka: 78638

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 5A, (nmr)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 933D, (ir)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 852B, (ir)

Sabatier, P. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1918, **158**, 834, (synth)

*Adv. Chem. Ser.*, 1955, **15**, 102, (*props*)

Seibl, J., *Arch. Mass Spectral Data*, 1970, **1**, 70, (ms)