



>>Entry Name: 4-(4-Methylphenyl)butanoic acid

Synonym(s): 4-Methylbenzenebutanoic acid, 9CI. 4-*p*-Tolylbutyric acid, 8CI

CAS Registry Number: 4521-22-6

Molecular Formula: C₁₁H₁₄O₂

Molecular Weight: 178.23

Accurate Mass: 178.09938

Percentage Composition: C 74.13%; H 7.92%; O 17.95%

Physical Description: Cryst. (petrol)

Melting Point: Mp 61-62° (57-58°)

Boiling Point: Bp_{0.4} 124-134° (lit. gives a pressure range)

Rare Chemicals Library: S53264-9

>>Derivative: Me ester

CAS Registry Number: 24306-23-8

Molecular Formula: C₁₂H₁₆O₂

Molecular Weight: 192.257

Accurate Mass: 192.11503

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

Physical Description: Oil

Boiling Point: Bp_{1.5} 84-86°

>>Derivative: Et ester

CAS Registry Number: 36440-63-8

Molecular Formula: C₁₃H₁₈O₂

Molecular Weight: 206.284

Accurate Mass: 206.13068

Percentage Composition: C 75.69%; H 8.79%; O 15.51%

Melting Point: Mp 40-41°

>>Derivative: Amide

Molecular Formula: C₁₁H₁₅NO

Molecular Weight: 177.246

Accurate Mass: 177.115364

Percentage Composition: C 74.54%; H 8.53%; N 7.90%; O 9.03%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 136.5°

References:

Durand, R., *Ann. Chim. (Paris)*, 1959, **4**, 45

Riout, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1965, 3312

Mathur, N.C. *et al.*, *Tetrahedron*, 1985, **41**, 1509, (*synth, deriv, pmr*)