



>>Entry Name: 2,4-Dibromobutanoic acid

CAS Registry Number: 63164-16-9

BrCH₂CH₂CHBrCOOH

Molecular Formula: C₄H₆Br₂O₂

Molecular Weight: 245.898

Accurate Mass: 243.913452

Percentage Composition: C 19.54%; H 2.46%; Br 64.99%; O 13.01%

>>Variant: (±)-form

Molecular Formula: C₄H₆Br₂O₂

Molecular Weight: 245.898

Accurate Mass: 243.913452

Percentage Composition: C 19.54%; H 2.46%; Br 64.99%; O 13.01%

Boiling Point: Bp₁₅ 130-131°

>>Derivative: Et ester

CAS Registry Number: 36847-51-5

Molecular Formula: C₆H₁₀Br₂O₂

Molecular Weight: 273.952

Accurate Mass: 271.944752

Percentage Composition: C 26.31%; H 3.68%; Br 58.33%; O 11.68%

Physical Description: Liq.

Boiling Point: Bp₅₂ 149°

Other: PB E07290

>>Derivative: Chloride

CAS Registry Number: 82820-87-9

Molecular Formula: C₄H₅Br₂ClO

Molecular Weight: 264.344

Accurate Mass: 261.879564

Percentage Composition: C 18.17%; H 1.91%; Br 60.45%; Cl 13.41%; O 6.05%

Boiling Point: Bp₁ 60-75°

>>Derivative: Amide

CAS Registry Number: 54882-37-0

Molecular Formula: C₄H₇Br₂NO

Molecular Weight: 244.913

Accurate Mass: 242.929436

Percentage Composition: C 19.62%; H 2.88%; Br 65.25%; N 5.72%; O 6.53%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 82°

Boiling Point: Subl._{0.1} 85°

>>Derivative: Nitrile

Molecular Formula: C₄H₅Br₂N

Molecular Weight: 226.898

Accurate Mass: 224.918871

Percentage Composition: C 21.17%; H 2.22%; Br 70.43%; N 6.17%

Physical Description: Liq.

References:

Nicolet, B.H. *et al.*, *J.A.C.S.*, 1927, **49**, 2066, (*synth*)

Wasserman, H.H. *et al.*, *J.O.C.*, 1981, **46**, 2991, (*Et ester*)

U.S. Pat., 1981, 4 247 468; *CA*, **94**, 174376h

Ikuta, H. *et al.*, *J. Med. Chem.*, 1987, **30**, 1995, (*chloride, amide, pmr*)

Brunet, P. *et al.*, *J.O.C.*, 1996, **61**, 2020, (*amide, nitrile, synth, ir, pmr, cmr*)