



Formula: C6H13NO2

MW: 131.17

CAS: 73-32-5

MDL: MFCD00004268

TNP: TNP00640

(2S,3S)-2-Amino-3-methylpentansaeure; (2s,3s)-alpha-amino-beta-merthylvalericacid;
(2s,3s)-alpha-amino-beta-methyl-n-valericacid; (s-(r*,r*)))-2-amino-3-methylpentanoicacaci;
(s-(r*,r*)))-2-amino-3-methylpentanoicacid; (S,S)-2-amino-3-methyl-pentanoicacid; (s,s)-iso



LogP: 2.23

LogS: -4.68

Acceptors: 2

Donors: 3

Rotation Bonds: 4

Chiral Centers: 2

N+O: 3

LIPINSKY: 4

IUPAC: isoleucine

Smiles: C(O)([C@H]([C@H](CC)(C))N)=O

Specification: Amino Acids; Isoleucine [Ile, I]; Amino Acids and Derivatives; alpha-Amino Acids; Biochemistry; Nutritional Supplements; Amino Acids (2S,3S)-2-Amino-3-methylpentanoic acid

Chemical Properties:

mp 288 C (dec.)(lit.) alpha 41