



Formula: C<sub>13</sub>H<sub>18</sub>O<sub>2</sub>

MW: 206.28

CAS: 15687-27-1

MDL NUMBER: MFCD00010393

IUPAC: 2-[4-(2-methylpropyl)phenyl]propanoic acid

Smiles: c1cc(ccc1CC(C)C)C(C(O)=O)C

THERAPEUTIC CATEGORY: Anti-inflammatory

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 3

N+O: 2

Chiral Centers: 1

LogP: 4.21

LogS: -4.11

LIPINSKI: 4

Synonyms: RARECHEM AL BO  
0989;MOTRIN(TM);(+/-)-2-(4-ISOBUTYLPHENYL)-PROPIONIC  
ACID;2-(4-ISOBUTYLPHENYL)PROPIONIC  
ACID;4-ISOBUTYL-ALPHA-METHYLPHENYLACETIC ACID;AKOS  
NCG1-0060;(+/-)-ALPHA-METHYL-4-(2-METHYLPROPYL)-BENZENEACETIC  
ACID;ALPHA-METHYL-4-[2-METHYLPROPYL]BENZENEACETIC ACID

CAS:15687-27-1

MF:C13H18O2

MW:206.28

EINECS:239-784-6

Product Categories:Active Pharmaceutical Ingredients;API;APIs;Inhibitors;Intermediates & Fine  
Chemicals;Pharmaceuticals;API's;Lipid signaling Ibuprofen

Chemical Properties: mp 77-78 C(lit.) bp 157 C (4 mmHg) Water Solubility insoluble Merck  
14,4881 Stability:Stable. Combustible. Incompatible with strong oxidizing agents.

CAS DataBase Reference: 15687-27-1(

CAS DataBase Reference: ) NIST Chemistry ReferenceIbuprofen(15687-27-1) EPA Substance  
Registry SystemBenzeneacetic acid, .alpha.-methyl-4-(2-methylpropyl)- (15687-27-1) Xn,N  
Risk Statements 22-63-51/53 Safety Statements 36-61-36/37 RIDADR 2811 WGK Germany 3  
RTECS MU6640000 HazardClass 6.1(b) PackingGroup III Hazardous Substances  
Data15687-27-1(Hazardous Substances Data) 2-(4-Isobutylphenyl)-propionic acid Ibuprofen

Usage And Synthesis:

Chemical Properties: Colourless, Crystalline Solid UsageA selective cyclooxygenase inhibitor  
(IC50=14.9uM). Inhibits PGH synthase-1 and PGH synthase-2 with comparable potency  
Ibuprofen

