



Formula: C<sub>10</sub>H<sub>14</sub>O<sub>2</sub>

MW: 166.22

CAS: 23635-14-5

Smiles: C1(C(=O)O)=CC[C@@H](C(=C)C)CC1

REFERENCE: 1. P.L. Crowell et al. J. Biol. Chem. 1991 266 17679

SOURCE: Naturally occurring monoiterpene found in essential oils of many fruits. Metabolyte of perillaldehyde, which isolated from *Perilla arguta*.

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 2

N+O: 2

Chiral Centers: 1

LogP: 3.27

LogS: -3.56

LIPINSKI: 4

Synonyms: 4-ISOPROPENYL-1-CYCLOHEXENE-1-CARBOXYLIC ACID;4-ISOPROPENYLCYCLOHEXENE-1-CARBOXYLIC ACID;L(-)-PERILLIC ACID;PERILLIC ACID;(S)-(-)-PERILLIC ACID;4-isopropenylcyclohex-1-enecarboxylic acid;4-prop-1-en-2-ylcyclohexene-1-carboxylic acid;4-(1-Methylvinyl)-1-cyclohexene-1-carboxylic acid

CAS:7694-45-3

MF:C10H14O2

MW:166.22

EINECS:231-709-5

Product Categories: PERILLIC ACID

Chemical Properties: mp 129-131 C(lit.) storage temp. 2-8C

CAS DataBase Reference: 7694-45-3(

CAS DataBase Reference: ) Xi Risk Statements 36/37/38 Safety Statements 26-36 WGK Germany 3 PERILLIC ACID

Usage And Synthesis: PERILLIC ACID

