



Formula: C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>

MW: 180.16

CAS: 50-78-2

MDL NUMBER: MFCD00002430

IUPAC: 2-acetyloxybenzoic acid

Smiles: c1(C(=O)O)c(OC(=O)C)cccc1

THERAPEUTIC CATEGORY: Analgesic, antipyretic, anti-inflammatory

ACCEPTORS: 4

DONORS: 1

ROTATION BONDS: 4

N+O: 4

Chiral Centers: 0

LogP: 1.6

LogS: -3.04

LIPINSKI: 4

Synonyms: Acetylsalicylic acid-a-13C;Aspirin-carboxyl-13C

CAS:

MF:13CC8H8O4

MW:0

EINECS:

Product Categories: Aspirin-carboxyl-13C

Chemical Properties: mp 134-136 C(lit.) Xn Risk Statements 22-36/37/38 Safety Statements 26 Aspirin-carboxyl-13C

Usage And Synthesis: Aspirin-carboxyl-13C

