

## Product Information

### Carbasalate calcium, Purity $\geq 98\%$

**Cat. No.:** X24-09-YM1426

**Size:** 50 mg; 100 mg; 200 mg; 500 mg

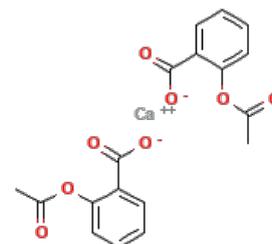
**CAS Number:** 5749-67-7

**Compound CID:** 21975

**Synonym:** 5749-67-7; Carbasalate Calcium; Iromin; Alcacyl; Omegin; Rheomin;

Solupsan; Calcium; 2-acetyloxybenzoate; urea

**This product is for research use only and is not intended for diagnostic use.**



#### Product Information

<b>Description</b>	Carbasalate calcium, soluble in DMSO and water and insoluble in ethanol, is a non-steroidal anti-inflammatory compound. The molecular weight of the compound is 458.436, and its molecular formula is $C_{19}H_{18}CaN_2O_9$ .
<b>Molecular Weight</b>	458.436
<b>Molecular Formula</b>	$C_{19}H_{18}CaN_2O_9$
<b>IUPAC Name</b>	Calcium;2-acetyloxybenzoate;urea
<b>InChI</b>	InChI=1S/2C9H8O4.CH4N2O.Ca/c2*1-6(10)13-8-5-3-2-4-7(8)9(11)12;2-1(3)4;/h2*2-5H,1H3,(H,11,12);(H4,2,3,4);/q;;;+2/p-2
<b>InChI Key</b>	VYMUGTALCSPLDM-UHFFFAOYSA-L
<b>Canonical SMILES</b>	<chem>CC(=O)OC1=CC=CC=C1C(=O)[O-].CC(=O)OC1=CC=CC=C1C(=O)[O-].C(=O)(N)N.[Ca+2]</chem>
<b>Isomeric SMILES</b>	<chem>CCCC(=O)O[C@@]1(CC[C@@H]2[C@@]1(C[C@@H]([C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)O)C(=O)COC(=O)CC</chem>
<b>Form</b>	Lyophilized powder
<b>Purity</b>	$\geq 98\%$
<b>Impurities</b>	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
<b>Solubility</b>	<i>In vitro</i> : DMSO: 10 mg/mL (21.81 mM); Water: 80 mg/mL (174.51 mM); Ethanol: insoluble
<b>Identity</b>	Confirmed by NMR/HPLC/MS.
<b>Stability</b>	In its lyophilized form, the chemical remains stable for 36 months.
<b>Quality Level</b>	Research grade
<b>Applications</b>	Carbasalate calcium can be studied extensively for its potential therapeutic applications in the



treatment of arthritis.

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**Storage**

Store at -20°C, and keep desiccated.

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