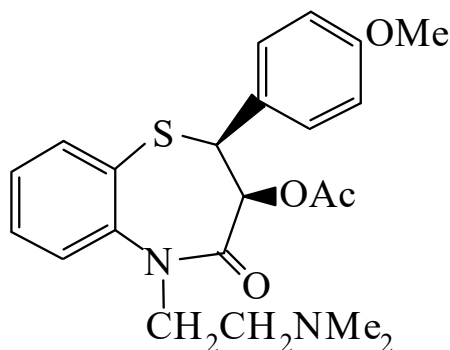




>>Entry Name: **Diltiazem**, BAN, INN

**Synonym(s):** 3-(Acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5*H*)-one, 9Cl. Adizem. Angiozem. Angitil. Calazem. Calcicard. Cardizem. Diacor. Dilzem. Latiazem. Slozem. Tiazac. Many other names



**CAS Registry Number:** 34933-06-7

**Extra CAS Registry Numbers(s):** 75472-92-3

**Type of Compound Code(s):** XA1650 XA7000 XA5210 XA2620 XA1020

**Molecular Formula:** C<sub>22</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>S

**Molecular Weight:** 414.524

**Accurate Mass:** 414.161328

**Percentage Composition:** C 63.75%; H 6.32%; N 6.76%; O 15.44%; S 7.74%

**Biological Use/Importance:** Coronary vasodilator, calcium antagonist. Antihypertensive and antianginal agent. Smooth muscle relaxant

**Development Status:** Marketed drug. Launched 1991

**Calculated Log P Data:** Log P 3.57 (uncertain value) (calc)

>>Variant: (2*S*,3*S*)-form

**Synonym(s):** (+)-*cis*-form

**CAS Registry Number:** 42399-41-7

**Molecular Formula:** C<sub>22</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>S

**Molecular Weight:** 414.524

**Accurate Mass:** 414.161328

**Percentage Composition:** C 63.75%; H 6.32%; N 6.76%; O 15.44%; S 7.74%

**Other Data:** *trans*-Isomers (2*R*,3*S*) and (2*S*,3*R*) have also been prepd. but show poor pharmacol. activity

>>Derivative: Hydrochloride

**Synonym(s):** **Diltiazem hydrochloride**, JAN, USAN. Anginyl. Herbesser. Blocalcin 60

**CAS Registry Number:** 33286-22-5

**Melting Point:** Mp 187-188°

**Solubility:** Insol. C<sub>6</sub>H<sub>6</sub>; sol. H<sub>2</sub>O, MeOH, CHCl<sub>3</sub>

**Experimental Log P Data:** Log P 2.7 (exp)

**Hazard & Toxicity:** LD<sub>50</sub> (rat, orl) 560 mg/kg

**Fluka:** 38489

**Sigma:** D2521

>>Derivative: *O*-De-Ac

**CAS Registry Number:** 42399-40-6

**Molecular Formula:** C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>S

**Molecular Weight:** 372.487

**Accurate Mass:** 372.150763

**Percentage Composition:** C 64.49%; H 6.49%; N 7.52%; O 12.89%; S 8.61%

**Metabolism:** Major metab. of Diltiazem in mammals

**Physical Description:** Gummy oil

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> +134.4 (c, 1 in CHCl<sub>3</sub>)

**References:**