

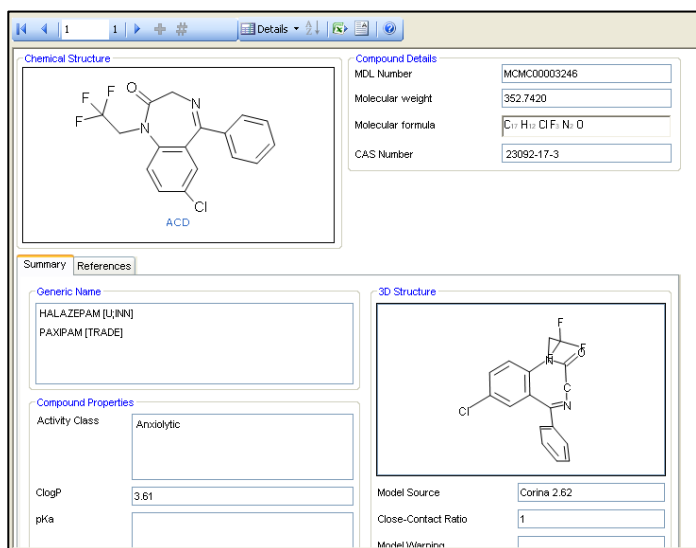
## Symyx Isentris Pharmacology Package

### For Smarter Lead Generation

Explore pharmacophores and lead compound structure-activity relationships, select scaffolds and R-groups for combinatorial libraries, compare ecotoxicology and biodegradation profiles, apply data about metabolic fate and toxic effects early in the discovery process, and monitor industry trends.

### Isentris provides rich functionality to access the Pharmacology databases:

- Drag-and-drop SAR table creation
- Rgroup decomposition for rapidly exploring the effects of substitution on the biological activity of a pharmacophore
- Citation hyper-linking to source literature information so scientists can obtain literature information without delay
- Customizable search, display, and report forms
- Metabolite explorer enabling researchers to explore known metabolite routes quickly.
- Automatic links in metabolic pathways to toxicity data indicating toxic metabolic intermediates
- Support for integration of in-house and Symyx databases so information can be searched as a single source
- Support for integration of content into existing scientific applications



**Chemical Structure**

**Compound Details**

MDL Number: MCMC00003246  
Molecular weight: 352.7420  
Molecular formula: C<sub>17</sub>H<sub>17</sub>ClF<sub>3</sub>N<sub>2</sub>O  
CAS Number: 23092-17-3

**Summary** | **References**

**Generic Name**

HALAZEPAM [UJNN]  
PAXIPAM [TRADE]

**Compound Properties**

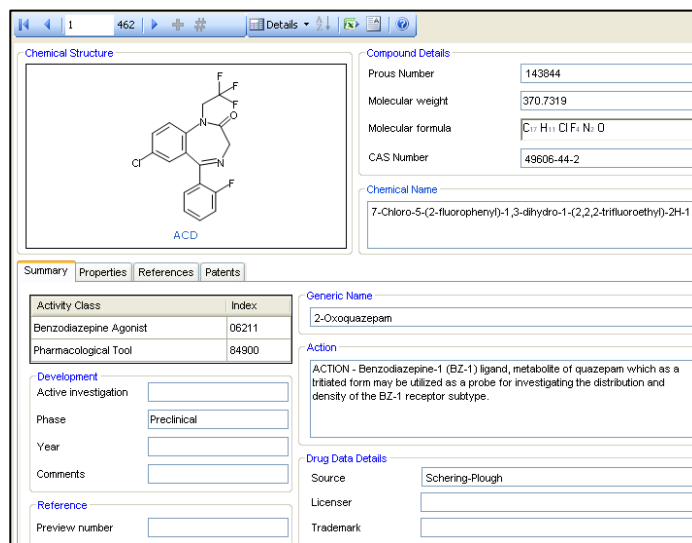
Activity Class: Anxiolytic

ClogP: 3.61  
pKa:

**3D Structure**

Model Source: Corina 2.62  
Close-Contact Ratio: 1  
Molwt Warning:

**MDDR:** Bioactivity information for newly launched and developing drugs



**Chemical Structure**

**Compound Details**

Prous Number: 143844  
Molecular weight: 370.7319  
Molecular formula: C<sub>17</sub>H<sub>14</sub>ClF<sub>3</sub>N<sub>2</sub>O  
CAS Number: 49606-44-2

**Chemical Name**

7-Chloro-5-(2-fluorophenyl)-1,3-dihydro-1-(2,2,2-trifluoroethyl)-2H-1,4-benzodiazepin-2-one

**Summary** | **Properties** | **References** | **Patents**

**Activity Class**

Activity Class	Index
Benzodiazepine Agonist	06211
Pharmacological Tool	84900

**Development**

Active Investigation:   
Phase: Preclinical  
Year:   
Comments:

**Reference**

Preview number:

**Generic Name**

2-Oxoquazepam

**Action**

ACTION - Benzodiazepine-1 (BZ-1) ligand, metabolite of quazepam which as a tritiated form may be utilized as a probe for investigating the distribution and density of the BZ-1 receptor subtype.

**Drug Data Details**

Source: Schering-Plough  
Licensor:   
Trademark:

**CMC:** Information on marketed and clinically studied drugs

Title	References
1-Poly(fluoroalkyl)benzodiazepines	<a href="#">Steinman, M. et al. J Med Chem 1973, 16(12): 1354. DOI: 10.1021/JM00270A008</a>
Use of the selective benzodiazepine-1 (BZ-1) ligand [3H]2-oxo-quazepam (SCH 15-725) to localize BZ-1 receptors in	<a href="#">Yezuita, J.P. et al. Neurosci Lett 1988, 86.</a>
Several new benzodiazepines selectively interact with a benzodiazepine receptor subtype	<a href="#">Siegwart, W. Neurosci Lett 1983, 38(1): 73. DOI: 10.1016/0304-3940(83)90113-1</a>
Time effects of food intake on the pharmacokinetics and pharmacodynamics of quazepam	<a href="#">Yasu-Furukori, N. et al. Br J Clin Pharmacol 2003, 55(4): 382. DOI: 10.1046/j.1365-2125.2003.01775.x</a>
Benzodiazepine receptor binding of benzodiazepine hypnotics: Receptor and ligand specificity	<a href="#">Miller, L.G. et al. Pharmacol Biochem Behav 1992, 43(2): 413. DOI: 10.1016/0091-3057(92)90170-K</a>
Effect of dietary fat content in meals on pharmacokinetics of quazepam	<a href="#">Yasu-Furukori, N. et al. J Clin Pharmacol 2002, 42(12): 1335. DOI: 10.1177/0091270002042012004</a>

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