

# Benzoximate

**Other names:**

Benzoic acid, anhydride with  
3-chloro-N-ethoxy-2,6-dimethoxybenzenecarboximidic acid  
Benzoic acid, anhydride with 3-chloro-N-ethoxy-2,6-dimethoxybenzimidic acid  
Benzomate  
Citrazon  
Benzohydroxamic acid, O-benzoyl-3-chloro-2,6-dimethoxy-N-ethyl-  
Acarbate  
Artaban  
Benzoic 3-chloro-N-ethoxy-2,6-dimethoxybenzimidic anhydride  
Benzoxamate  
Ethyl O-benzoyl 3-chloro-2,6-dimethoxy-benzohydroximate  
NA-53  
Benzimidic acid, 3-chloro-N-ethoxy-2,6-dimethoxy-, anhydride with benzoic acid  
Ethyl O-benzoyl-3-chloro-2,6-dimethoxybenzohydroxamate  
Aazomate  
(3-Chloro-2,6-dimethoxyphenyl)(ethoxyimino)methyl benzoate

**Inchi:**

InChI=1S/C18H18ClNO5/c1-4-24-20-17(25-18(21)12-8-6-5-7-9-12)15-14(22-2)11-10-13(

**InchiKey:**

BZMIHNKNQJVVRO-UHFFFAOYSA-N

**Formula:**

C18H18ClNO5

**SMILES:**

CCON=C(OC(=O)c1cccc1)c1c(OC)ccc(Cl)c1OC

**Mol. weight [g/mol]:**

363.79

**CAS:**

29104-30-1

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -560.97 | kJ/mol | Joback Method  |
| hvap          | 86.36   | kJ/mol | Joback Method  |
| log10ws       | -4.93   |        | Crippen Method |
| logp          | 3.912   |        | Crippen Method |
| mcvol         | 259.930 | ml/mol | McGowan Method |
| pc            | 1637.78 | kPa    | Joback Method  |
| tb            | 937.08  | K      | Joback Method  |
| tc            | 1175.25 | K      | Joback Method  |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C29104301&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29104301&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>   |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |

# Legend

|                 |   |
|-----------------|---|
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |

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