# Cyclandelate

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|---|---|
| **Other names:** | Benzeneacetic acid, «alpha»-hydroxy-, 3,3,5-trimethylcyclohexyl ester |
| | Mandelic acid, 3,3,5-trimethylcyclohexyl ester |
| | Arto-espasmol |
| | BS 572 |
| | Capilan |
| | Ciclospasmol |
| | Clandilon |
| | Cyclolyt |
| | Cyclomandol |
| | Cyclospasmol |
| | Dilatan |
| | «alpha»-Hydroxybenzeneacetic acid 3,3,5-trimethylcyclohexyl ester |
| | Perebral |
| | Saiclate |
| | Sancyclan |
| | Sepyron |
| | Spasmione |
| | Spasmocyclon |
| | Spasmocyclone |
| | 3,3,5-Trimethylcyclohexanol «alpha»-phenyl-«alpha»-hydroxyacetate |
| | 3,5,5-Trimethylcyclohexyl amygdalate |
| | 3,3,5-Trimethylcyclohexyl mandelate |
| | Cyclergine |
| | Cyclobral |
| | Natil |
| | Novodil |
| | 3,5,5-Trimethylcyclohexanol, mandelic acid ester |
| | 3,5,5-Trimethylcyclohexyl mandelate |
| **Inchi:** | InChI=1S/C17H24O3/c1-12-9-14(11-17(2,3)10-12)20-16(19)15(18)13-7-5-4-6-8-13/h4-8, |
| **InchiKey:** | WZHCOOQXZCIUNC-UHFFFAOYSA-N |
| **Formula:** | C17H24O3 |
| **SMILES:** | CC1CC(OC(=O)C(O)c2ccccc2)CC(C)(C)C1 |
| **Mol. weight [g/mol]:** | 276.37 |
| **CAS:** | 456-59-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|

| | | | |
|---|---|---|---|
| gf | -164.97 | kJ/mol | Joback Method |
| hf | -531.11 | kJ/mol | Joback Method |
| hfus | 24.86 | kJ/mol | Joback Method |
| hvap | 79.82 | kJ/mol | Joback Method |
| log10ws | -4.15 | | Crippen Method |
| logp | 3.478 | | Crippen Method |
| mcvol | 229.080 | ml/mol | McGowan Method |
| pc | 2086.93 | kPa | Joback Method |
| rinpol | 1903.00 | | NIST Webbook |
| rinpol | 1890.00 | | NIST Webbook |
| tb | 793.52 | K | Joback Method |
| tc | 1012.08 | K | Joback Method |
| tf | 448.55 | K | Joback Method |
| vc | 0.846 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 717.44 | J/mol×K | 793.52 | Joback Method |
| cpg | 735.40 | J/mol×K | 829.95 | Joback Method |
| cpg | 752.54 | J/mol×K | 866.37 | Joback Method |
| cpg | 768.97 | J/mol×K | 902.80 | Joback Method |
| cpg | 784.83 | J/mol×K | 939.23 | Joback Method |
| cpg | 800.21 | J/mol×K | 975.66 | Joback Method |
| cpg | 815.26 | J/mol×K | 1012.08 | Joback Method |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C456597&Units=SI

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |