# ETHYLBENZOYLECGONINE

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|---|---|
| **Other names:** | [1R-(Exo,exo)]-3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylateacid |
| | Cocaethylene |
| | Ethylbenzoylecgonine |
| | Homocaine |
| | thylbenzoylecgonine (cocaethylene) |
| **Inchi:** | InChI=1S/C18H23NO4/c1-3-22-18(21)16-14-10-9-13(19(14)2)11-15(16)23-17(20)12-7-5- |
| **InchiKey:** | NMPOSNRHZIWLLL-UHFFFAOYSA-N |
| **Formula:** | C18H23NO4 |
| **SMILES:** | CCOC(=O)C1C(OC(=O)c2ccccc2)CC2CCC1N2C |
| **Mol. weight [g/mol]:** | 317.38 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6622 | | Cheméo Relay (1.0) |
| hvap | 108.95 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.40 | eV | Cheméo Relay (1.0) |
| log10ws | -2.28 | | Cheméo Relay (1.0) |
| logp | 2.258 | | Crippen Method |
| mcvol | 243.860 | ml/mol | McGowan Method |
| pc | 1512.98 | kPa | Cheméo Relay (1.0, beta) |
| rinpol | 2219.00 | | NIST Webbook |
| rinpol | 2219.00 | | NIST Webbook |
| rinpol | 2219.00 | | NIST Webbook |
| tb | 634.24 | K | Cheméo Relay (1.0) |
| tc | 903.69 | K | Cheméo Relay (1.0) |
| tf | 384.08 | K | Cheméo Relay (1.0) |

## Sources

| | |
|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C529384&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |

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