# 2-Carbomethoxyphenyl isocyanate

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|---|---|
| **Other names:** | 2-Methoxycarbonylphenyl isocyanate |
| **Inchi:** | InChI=1S/C9H7NO3/c1-13-9(12)7-4-2-3-5-8(7)10-6-11/h2-5H,1H3 |
| **InchiKey:** | ATFKBWNEVZUSKC-UHFFFAOYSA-N |
| **Formula:** | C9H7NO3 |
| **SMILES:** | COC(=O)c1ccccc1N=C=O |
| **Mol. weight [g/mol]:** | 177.16 |
| **CAS:** | 1793-07-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -254.24 | kJ/mol | Joback Method |
| hvap | 57.25 | kJ/mol | Joback Method |
| log10ws | -6.20 | | Crippen Method |
| logp | 1.440 | | Crippen Method |
| mcvol | 128.600 | ml/mol | McGowan Method |
| pc | 3690.97 | kPa | Joback Method |
| tb | 579.94 | K | Joback Method |
| tc | 804.54 | K | Joback Method |

# Sources

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|---|---|
| **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=C1793073&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |

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