# Benzene, 1-isocyanato-2-methoxy-

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|---|---|
| **Other names:** | 2-Methoxyphenylisocyanate |
| | o-Methoxyphenyl isocyanate |
| **Inchi:** | InChI=1S/C8H7NO2/c1-11-8-5-3-2-4-7(8)9-6-10/h2-5H,1H3 |
| **InchiKey:** | SUVCZZADQDCIEQ-UHFFFAOYSA-N |
| **Formula:** | C8H7NO2 |
| **SMILES:** | COc1ccccc1N=C=O |
| **Mol. weight [g/mol]:** | 149.15 |
| **CAS:** | 700-87-8 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -121.02 | kJ/mol | Joback Method |
| hvap | 48.28 | kJ/mol | Joback Method |
| log10ws | -6.07 | | Crippen Method |
| logp | 1.662 | | Crippen Method |
| mcvol | 112.940 | ml/mol | McGowan Method |
| pc | 3843.54 | kPa | Joback Method |
| tb | 503.19 | K | Joback Method |
| tc | 723.14 | K | Joback Method |

## Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C700878&Units=SI |
| **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 |

## Legend

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

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |