# Benzoic acid, 3-iodo-, methyl ester

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|---|---|
| **Other names:** | Benzoic acid, m-iodo-, methyl ester |
| | Methyl m-iodobenzoate |
| | Methyl 3-iodobenzoate |
| | 3-Iodomethylbenzoate |
| **Inchi:** | InChI=1S/C8H7IO2/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5H,1H3 |
| **InchiKey:** | NPXOIGSBRLCOSD-UHFFFAOYSA-N |
| **Formula:** | C8H7IO2 |
| **SMILES:** | COC(=O)c1cccc(I)c1 |
| **Mol. weight [g/mol]:** | 262.04 |
| **CAS:** | 618-91-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3870.20 ± 4.20 | kJ/mol | NIST Webbook |
| gf | -56.54 | kJ/mol | Joback Method |
| hf | -151.32 | kJ/mol | Joback Method |
| hfus | 17.32 | kJ/mol | Joback Method |
| hvap | 54.87 | kJ/mol | Joback Method |
| log10ws | -2.86 | | Crippen Method |
| logp | 2.078 | | Crippen Method |
| mcvol | 133.080 | ml/mol | McGowan Method |
| pc | 3690.97 | kPa | Joback Method |
| rinpol | 1448.00 | | NIST Webbook |
| rinpol | 1448.00 | | NIST Webbook |
| tb | 583.53 | K | Joback Method |
| tc | 836.60 | K | Joback Method |
| tf | 349.08 | K | Joback Method |
| vc | 0.487 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 255.67 | J/mol×K | 583.53 | Joback Method |
| cpg | 265.96 | J/mol×K | 625.71 | Joback Method |

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|---|---|---|---|---|
| cpg | 275.50 | J/mol×K | 667.89 | Joback Method |
| cpg | 284.30 | J/mol×K | 710.06 | Joback Method |
| cpg | 292.40 | J/mol×K | 752.24 | Joback Method |
| cpg | 299.81 | J/mol×K | 794.42 | Joback Method |
| cpg | 306.58 | J/mol×K | 836.60 | Joback Method |
| dvisc | 0.0019750 | Pa×s | 349.08 | Joback Method |
| dvisc | 0.0011856 | Pa×s | 388.16 | Joback Method |
| dvisc | 0.0007813 | Pa×s | 427.23 | Joback Method |
| dvisc | 0.0005522 | Pa×s | 466.31 | Joback Method |
| dvisc | 0.0004118 | Pa×s | 505.38 | Joback Method |
| dvisc | 0.0003203 | Pa×s | 544.45 | Joback Method |
| dvisc | 0.0002576 | Pa×s | 583.53 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 549.70 | K | 98.50 | NIST Webbook |
| tbrp | 423.20 | K | 2.40 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C618917&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**chs:** Standard solid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |