# Benzoic acid, 4-iodo-, methyl ester

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|---|---|
| **Other names:** | Benzoic acid, p-iodo-, methyl ester |
| | Methyl 4-iodobenzoate |
| | Methyl p-iodobenzoate |
| **Inchi:** | InChI=1S/C8H7IO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,1H3 |
| **InchiKey:** | DYUWQWMXZHDZOR-UHFFFAOYSA-N |
| **Formula:** | C8H7IO2 |
| **SMILES:** | COC(=O)c1ccc(I)cc1 |
| **Mol. weight [g/mol]:** | 262.04 |
| **CAS:** | 619-44-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3861.80 ± 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 |
| ie | 9.10 | eV | NIST Webbook |
| ie | 8.73 | eV | NIST Webbook |
| log10ws | -2.86 | | Crippen Method |
| logp | 2.078 | | Crippen Method |
| mcvol | 133.080 | ml/mol | McGowan Method |
| pc | 3690.97 | kPa | Joback Method |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| tb | 583.53 | K | Joback Method |
| tc | 836.60 | K | Joback Method |
| tf | 386.67 | K | The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids |
| 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 |
| 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 |

# 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=C619443&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids:** | https://www.doi.org/10.1016/j.jct.2012.07.027 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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

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|---|---|
| **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 |
| **vc:** | Critical Volume |