# trans Methyl 3-iodo-2-propenoate

**Inchi:** InChI=1S/C4H5IO2/c1-7-4(6)2-3-5/h2-3H,1H3/b3-2+
**InchiKey:** SUQXOFVGKSUSSM-NSCUHMNNSA-N
**Formula:** C4H5IO2
**SMILES:** COC(=O)C=CI
**Mol. weight [g/mol]:** 211.99
**CAS:** 6213-88-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -112.78 | kJ/mol | Joback Method |
| hf | -176.60 | kJ/mol | Joback Method |
| hfus | 13.51 | kJ/mol | Joback Method |
| hvap | 42.98 | kJ/mol | Joback Method |
| log10ws | -1.66 | | Crippen Method |
| logp | 1.108 | | Crippen Method |
| mcvol | 96.180 | ml/mol | McGowan Method |
| pc | 4294.29 | kPa | Joback Method |
| tb | 464.51 | K | Joback Method |
| tc | 691.60 | K | Joback Method |
| tf | 259.98 | K | Joback Method |
| vc | 0.351 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 149.47 | J/mol×K | 464.51 | Joback Method |
| cpg | 155.98 | J/mol×K | 502.36 | Joback Method |
| cpg | 162.09 | J/mol×K | 540.21 | Joback Method |
| cpg | 167.82 | J/mol×K | 578.06 | Joback Method |
| cpg | 173.19 | J/mol×K | 615.90 | Joback Method |
| cpg | 178.22 | J/mol×K | 653.75 | Joback Method |
| cpg | 182.93 | J/mol×K | 691.60 | Joback Method |
| dvisc | 0.0034362 | Pa×s | 259.98 | Joback Method |
| dvisc | 0.0018514 | Pa×s | 294.07 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0011343 | Pa×s | 328.16 | Joback Method |
| dvisc | 0.0007620 | Pa×s | 362.25 | Joback Method |
| dvisc | 0.0005482 | Pa×s | 396.33 | Joback Method |
| dvisc | 0.0004155 | Pa×s | 430.42 | Joback Method |
| dvisc | 0.0003280 | Pa×s | 464.51 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6213883&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

| | |
|---|---|
| **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 |
| **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 |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |