# o-Toluic acid, 3-chloropen-2-enyl ester

**Other names:** o-Toluylic acid, 3-chloropen-2-enyl ester
**Inchi:** InChI=1S/C11H11ClO2/c1-9-5-2-3-6-10(9)11(13)14-8-4-7-12/h2-7H,8H2,1H3/b7-4+
**InchiKey:** MKXZDOUAKCYRJS-QPJJXVBHSA-N
**Formula:** C11H11ClO2
**SMILES:** Cc1ccccc1C(=O)OCC=CCl
**Mol. weight [g/mol]:** 210.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -21.11 | kJ/mol | Joback Method |
| hf | -188.63 | kJ/mol | Joback Method |
| hfus | 25.08 | kJ/mol | Joback Method |
| hvap | 56.52 | kJ/mol | Joback Method |
| log10ws | -3.53 | | Crippen Method |
| logp | 2.904 | | Crippen Method |
| mcvol | 157.470 | ml/mol | McGowan Method |
| pc | 2778.85 | kPa | Joback Method |
| rinpol | 1585.90 | | NIST Webbook |
| tb | 600.62 | K | Joback Method |
| tc | 824.35 | K | Joback Method |
| tf | 349.67 | K | Joback Method |
| vc | 0.597 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 352.29 | J/mol×K | 600.62 | Joback Method |
| cpg | 364.97 | J/mol×K | 637.91 | Joback Method |
| cpg | 376.83 | J/mol×K | 675.20 | Joback Method |
| cpg | 387.90 | J/mol×K | 712.49 | Joback Method |
| cpg | 398.21 | J/mol×K | 749.77 | Joback Method |
| cpg | 407.80 | J/mol×K | 787.06 | Joback Method |
| cpg | 416.70 | J/mol×K | 824.35 | Joback Method |
| dvisc | 0.0014831 | Pa×s | 349.67 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0008442 | Pa×s | 391.50 | Joback Method |
| dvisc | 0.0005358 | Pa×s | 433.32 | Joback Method |
| dvisc | 0.0003684 | Pa×s | 475.14 | Joback Method |
| dvisc | 0.0002691 | Pa×s | 516.97 | Joback Method |
| dvisc | 0.0002060 | Pa×s | 558.79 | Joback Method |
| dvisc | 0.0001637 | Pa×s | 600.62 | 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=U292518&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |