# tert-Butyl 2,4,5-trichlorophenyl carbonate

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|---|---|
| **Other names:** | t-Butyl 2,4,5-trichlorophenyl carbonate |
| | Carbonic acid, 1,1-dimethylethyl 2,4,5-trichlorophenyl ester |
| **Inchi:** | InChI=1S/C11H11Cl3O3/c1-11(2,3)17-10(15)16-9-5-7(13)6(12)4-8(9)14/h4-5H,1-3H3 |
| **InchiKey:** | LJFPGBIHDPZHIN-UHFFFAOYSA-N |
| **Formula:** | C11H11Cl3O3 |
| **SMILES:** | CC(C)(C)OC(=O)Oc1cc(Cl)c(Cl)cc1Cl |
| **Mol. weight [g/mol]:** | 297.56 |
| **CAS:** | 16965-08-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -246.61 | kJ/mol | Joback Method |
| hf | -501.24 | kJ/mol | Joback Method |
| hfus | 26.27 | kJ/mol | Joback Method |
| hvap | 67.77 | kJ/mol | Joback Method |
| log10ws | -5.27 | | Crippen Method |
| logp | 4.961 | | Crippen Method |
| mcvol | 192.120 | ml/mol | McGowan Method |
| pc | 2377.22 | kPa | Joback Method |
| tb | 700.47 | K | Joback Method |
| tc | 932.89 | K | Joback Method |
| tf | 464.28 | K | Joback Method |
| vc | 0.722 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 445.75 | J/mol×K | 700.47 | Joback Method |
| cpg | 457.01 | J/mol×K | 739.21 | Joback Method |
| cpg | 467.42 | J/mol×K | 777.94 | Joback Method |
| cpg | 476.99 | J/mol×K | 816.68 | Joback Method |
| cpg | 485.74 | J/mol×K | 855.42 | Joback Method |
| cpg | 493.69 | J/mol×K | 894.15 | Joback Method |
| cpg | 500.86 | J/mol×K | 932.89 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0006395 | Pa×s | 464.28 | Joback Method |
| dvisc | 0.0004219 | Pa×s | 503.64 | Joback Method |
| dvisc | 0.0002956 | Pa×s | 543.01 | Joback Method |
| dvisc | 0.0002174 | Pa×s | 582.38 | Joback Method |
| dvisc | 0.0001662 | Pa×s | 621.74 | Joback Method |
| dvisc | 0.0001312 | Pa×s | 661.11 | Joback Method |
| dvisc | 0.0001063 | Pa×s | 700.47 | 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=C16965085&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **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 |