# 2,4,6-Tribromo-3-chloroanisole

**Inchi:** InChI=1S/C7H4Br3ClO/c1-12-7-4(9)2-3(8)6(11)5(7)10/h2H,1H3
**InchiKey:** FWKUBDOTUFVPBX-UHFFFAOYSA-N
**Formula:** C7H4Br3ClO
**SMILES:** COc1c(Br)cc(Br)c(Cl)c1Br
**Mol. weight [g/mol]:** 379.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 7.98 | kJ/mol | Joback Method |
| hf | -66.13 | kJ/mol | Joback Method |
| hfus | 27.61 | kJ/mol | Joback Method |
| hvap | 62.20 | kJ/mol | Joback Method |
| log10ws | -5.77 | | Crippen Method |
| logp | 4.636 | | Crippen Method |
| mcvol | 156.340 | ml/mol | McGowan Method |
| pc | 4652.99 | kPa | Joback Method |
| rinpol | 1846.00 | | NIST Webbook |
| rinpol | 1846.00 | | NIST Webbook |
| tb | 664.49 | K | Joback Method |
| tc | 931.38 | K | Joback Method |
| tf | 476.70 | K | Joback Method |
| vc | 0.573 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 263.71 | J/mol×K | 664.49 | Joback Method |
| cpg | 270.50 | J/mol×K | 708.97 | Joback Method |
| cpg | 276.79 | J/mol×K | 753.45 | Joback Method |
| cpg | 282.59 | J/mol×K | 797.94 | Joback Method |
| cpg | 287.95 | J/mol×K | 842.42 | Joback Method |
| cpg | 292.89 | J/mol×K | 886.90 | Joback Method |
| cpg | 297.44 | J/mol×K | 931.38 | Joback Method |
| dvisc | 0.0006380 | Pa×s | 476.70 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004961 | Pa×s | 508.00 | Joback Method |
| dvisc | 0.0003973 | Pa×s | 539.30 | Joback Method |
| dvisc | 0.0003259 | Pa×s | 570.60 | Joback Method |
| dvisc | 0.0002730 | Pa×s | 601.89 | Joback Method |
| dvisc | 0.0002327 | Pa×s | 633.19 | Joback Method |
| dvisc | 0.0002013 | Pa×s | 664.49 | Joback Method |

# Sources

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|---|---|
| **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=R323507&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |