# METHYL 4-TERT-BUTYL-DITHIABENZOATE

**Other names:** Methyl 4-tert-butylbenzenecarbodithioate
Benzenecarbodithioic acid, 4-(1,1-dimethylethyl)-, methyl ester
**Inchi:** InChI=1S/C12H16S2/c1-12(2,3)10-7-5-9(6-8-10)11(13)14-4/h5-8H,1-4H3
**InchiKey:** XGVNDLXEGXTPBM-UHFFFAOYSA-N
**Formula:** C12H16S2
**SMILES:** CSC(=S)c1ccc(C(C)(C)C)cc1
**Mol. weight [g/mol]:** 224.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 12.14 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 21.81 | kJ/mol | Joback Method |
| hvap | 92.00 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.99 | eV | Cheméo Relay (1.0) |
| log10ws | -5.70 | | Cheméo Relay (1.0) |
| logp | 4.023 | | Crippen Method |
| mcvol | 184.580 | ml/mol | McGowan Method |
| pc | 2695.80 | kPa | Joback Method |
| tb | 562.32 | K | Cheméo Relay (1.0) |
| tc | 781.32 | K | Cheméo Relay (1.0) |
| tf | 352.19 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 440.27 | J/mol×K | 641.21 | Joback Method |
| cpg | 455.99 | J/mol×K | 684.27 | Joback Method |
| cpg | 470.40 | J/mol×K | 727.33 | Joback Method |
| cpg | 483.63 | J/mol×K | 770.39 | Joback Method |
| cpg | 495.81 | J/mol×K | 813.45 | Joback Method |
| cpg | 507.08 | J/mol×K | 856.51 | Joback Method |
| cpg | 517.58 | J/mol×K | 899.57 | 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 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C58863426&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |