# 4-sec-Butyl-2-tert-butyl-6-hydroperoxymethyl-phe

**Inchi:** InChI=1S/C15H24O3/c1-6-10(2)11-7-12(9-18-17)14(16)13(8-11)15(3,4)5/h7-8,10,16-17H
**InchiKey:** HVMLPRKOWGHNKO-UHFFFAOYSA-N
**Formula:** C15H24O3
**SMILES:** CCC(C)c1cc(COO)c(O)c(C(C)(C)C)c1
**Mol. weight [g/mol]:** 252.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -329.56 | kJ/mol | Joback Method |
| hf | -680.95 | kJ/mol | Joback Method |
| hfus | 32.86 | kJ/mol | Joback Method |
| hvap | 81.08 | kJ/mol | Joback Method |
| log10ws | -4.22 | | Crippen Method |
| logp | 4.193 | | Crippen Method |
| mcvol | 216.060 | ml/mol | McGowan Method |
| pc | 2151.31 | kPa | Joback Method |
| rinpol | 1753.00 | | NIST Webbook |
| rinpol | 1753.00 | | NIST Webbook |
| tb | 801.70 | K | Joback Method |
| tc | 1028.56 | K | Joback Method |
| tf | 570.01 | K | Joback Method |
| vc | 0.741 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 637.15 | J/mol×K | 801.70 | Joback Method |
| cpg | 651.08 | J/mol×K | 839.51 | Joback Method |
| cpg | 664.30 | J/mol×K | 877.32 | Joback Method |
| cpg | 676.94 | J/mol×K | 915.13 | Joback Method |
| cpg | 689.11 | J/mol×K | 952.94 | Joback Method |
| cpg | 700.93 | J/mol×K | 990.75 | Joback Method |
| cpg | 712.54 | J/mol×K | 1028.56 | Joback Method |
| dvisc | 0.0000770 | Pa×s | 570.01 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000431 | Pa×s | 608.62 | Joback Method |
| dvisc | 0.0000258 | Pa×s | 647.24 | Joback Method |
| dvisc | 0.0000164 | Pa×s | 685.86 | Joback Method |
| dvisc | 0.0000109 | Pa×s | 724.47 | Joback Method |
| dvisc | 0.0000076 | Pa×s | 763.09 | Joback Method |
| dvisc | 0.0000055 | Pa×s | 801.70 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R169878&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |