# 2-tert-Butyl-4-methyl-6-(a-methylbenzyl)phenol

**Other names:** 2-tert-butyl-4-methyl-6-«alpha»-methylbenzylphenol
**Inchi:** InChI=1S/C19H24O/c1-13-11-16(14(2)15-9-7-6-8-10-15)18(20)17(12-13)19(3,4)5/h6-12,
**InchiKey:** KYWXWCOPNNMDMN-UHFFFAOYSA-N
**Formula:** C19H24O
**SMILES:** Cc1cc(C(C)c2ccccc2)c(O)c(C(C)(C)C)c1
**Mol. weight [g/mol]:** 268.39
**CAS:** 1706-65-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 160.44 | kJ/mol | Joback Method |
| hf | -176.71 | kJ/mol | Joback Method |
| hfus | 27.12 | kJ/mol | Joback Method |
| hvap | 75.09 | kJ/mol | Joback Method |
| log10ws | -5.29 | | Crippen Method |
| logp | 5.150 | | Crippen Method |
| mcvol | 236.920 | ml/mol | McGowan Method |
| pc | 2003.70 | kPa | Joback Method |
| tb | 774.39 | K | Joback Method |
| tc | 1017.45 | K | Joback Method |
| tf | 338.00 ± 0.20 | K | NIST Webbook |
| vc | 0.833 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 786.77 | J/mol×K | 1017.45 | Joback Method |
| cpg | 772.92 | J/mol×K | 976.94 | Joback Method |
| cpg | 758.61 | J/mol×K | 936.43 | Joback Method |
| cpg | 743.69 | J/mol×K | 895.92 | Joback Method |
| cpg | 727.99 | J/mol×K | 855.41 | Joback Method |
| cpg | 711.33 | J/mol×K | 814.90 | Joback Method |
| cpg | 693.55 | J/mol×K | 774.39 | Joback Method |
| dvisc | 0.0002527 | Pa×s | 480.91 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000055 | Pa×s | 774.39 | Joback Method |
| dvisc | 0.0000084 | Pa×s | 725.48 | Joback Method |
| dvisc | 0.0000136 | Pa×s | 676.56 | Joback Method |
| dvisc | 0.0000239 | Pa×s | 627.65 | Joback Method |
| dvisc | 0.0000459 | Pa×s | 578.74 | Joback Method |
| dvisc | 0.0000995 | Pa×s | 529.82 | Joback Method |
| hfust | 31.38 | kJ/mol | 337.70 | NIST Webbook |

# Sources

| | |
|---|---|
| **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=C1706656&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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |