# Benzenepropanal, 4-(1,1-dimethylethyl)-

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|---|---|
| **Other names:** | Bourgeonal |
| | p-tert-Butyldihydrocinnamaldehyde |
| | 4-(1,1-Dimethylethyl)benzenepropanal |
| | p-tert-Butyl phenylpropyl-aldehyde 1 |
| | 3-(4-tert-butylphenyl)propionaldehyde |
| | Propanal, 3-(4-(1,1-dimethylethyl)phenyl) |
| **Inchi:** | InChI=1S/C13H18O/c1-13(2,3)12-8-6-11(7-9-12)5-4-10-14/h6-10H,4-5H2,1-3H3 |
| **InchiKey:** | FZJUFJKVIYFBSY-UHFFFAOYSA-N |
| **Formula:** | C13H18O |
| **SMILES:** | CC(C)(C)c1ccc(CCC=O)cc1 |
| **Mol. weight [g/mol]:** | 190.28 |
| **CAS:** | 18127-01-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 64.68 | kJ/mol | Joback Method |
| hf | -180.92 | kJ/mol | Joback Method |
| hfus | 17.95 | kJ/mol | Joback Method |
| hvap | 52.89 | kJ/mol | Joback Method |
| log10ws | -3.29 | | Crippen Method |
| logp | 3.116 | | Crippen Method |
| mcvol | 171.840 | ml/mol | McGowan Method |
| pc | 2363.37 | kPa | Joback Method |
| rinpol | 1212.00 | | NIST Webbook |
| rinpol | 1212.00 | | NIST Webbook |
| ripol | 2030.00 | | NIST Webbook |
| ripol | 2030.00 | | NIST Webbook |
| tb | 573.93 | K | Joback Method |
| tc | 787.33 | K | Joback Method |
| tf | 319.63 | K | Joback Method |
| vc | 0.661 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 420.39 | J/mol×K | 573.93 | Joback Method |
| cpg | 436.90 | J/mol×K | 609.50 | Joback Method |
| cpg | 452.34 | J/mol×K | 645.06 | Joback Method |
| cpg | 466.78 | J/mol×K | 680.63 | Joback Method |
| cpg | 480.26 | J/mol×K | 716.20 | Joback Method |
| cpg | 492.85 | J/mol×K | 751.77 | Joback Method |
| cpg | 504.61 | J/mol×K | 787.33 | Joback Method |
| dvisc | 0.0030332 | Pa×s | 319.63 | Joback Method |
| dvisc | 0.0014850 | Pa×s | 362.01 | Joback Method |
| dvisc | 0.0008444 | Pa×s | 404.40 | Joback Method |
| dvisc | 0.0005345 | Pa×s | 446.78 | Joback Method |
| dvisc | 0.0003662 | Pa×s | 489.16 | Joback Method |
| dvisc | 0.0002665 | Pa×s | 531.55 | Joback Method |
| dvisc | 0.0002032 | Pa×s | 573.93 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C18127010&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

# 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
**ripol:** Polar retention indices

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|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |