# Benzaldehyde, 4-(heptyloxy)-

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|---|---|
| **Other names:** | 4-n-Heptyloxybenzaldehyde |
| | 4-(Heptyloxy)benzaldehyde |
| | p-Heptyloxybenzaldehyde |
| | p-n-Heptoxybenzaldehyde |
| | 4-n-Heptoxybenzaldehyde |
| | p-n-Heptyloxybenzaldehyde |
| **Inchi:** | InChI=1S/C14H20O2/c1-2-3-4-5-6-11-16-14-9-7-13(12-15)8-10-14/h7-10,12H,2-6,11H2,1 |
| **InchiKey:** | YBCKMIZXHKVONZ-UHFFFAOYSA-N |
| **Formula:** | C14H20O2 |
| **SMILES:** | CCCCCCCOc1ccc(C=O)cc1 |
| **Mol. weight [g/mol]:** | 220.31 |
| **CAS:** | 27893-41-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -34.74 | kJ/mol | Joback Method |
| hf | -325.03 | kJ/mol | Joback Method |
| hfus | 29.14 | kJ/mol | Joback Method |
| hvap | 58.83 | kJ/mol | Joback Method |
| log10ws | -4.34 | | Crippen Method |
| logp | 3.848 | | Crippen Method |
| mcvol | 191.800 | ml/mol | McGowan Method |
| pc | 2086.93 | kPa | Joback Method |
| tb | 622.46 | K | Joback Method |
| tc | 819.31 | K | Joback Method |
| tf | 350.71 | K | Joback Method |
| vc | 0.747 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 493.99 | J/mol×K | 622.46 | Joback Method |
| cpg | 564.88 | J/mol×K | 786.51 | Joback Method |
| cpg | 552.29 | J/mol×K | 753.70 | Joback Method |

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|---|---|---|---|---|
| cpg | 538.93 | J/mol×K | 720.89 | Joback Method |
| cpg | 524.77 | J/mol×K | 688.08 | Joback Method |
| cpg | 509.80 | J/mol×K | 655.27 | Joback Method |
| cpg | 576.71 | J/mol×K | 819.31 | Joback Method |
| dvisc | 0.0001650 | Pa×s | 622.46 | Joback Method |
| dvisc | 0.0002104 | Pa×s | 577.17 | Joback Method |
| dvisc | 0.0002795 | Pa×s | 531.88 | Joback Method |
| dvisc | 0.0003914 | Pa×s | 486.59 | Joback Method |
| dvisc | 0.0005876 | Pa×s | 441.29 | Joback Method |
| dvisc | 0.0009678 | Pa×s | 396.00 | Joback Method |
| dvisc | 0.0018135 | Pa×s | 350.71 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 426.00 ± 1.00 | K | 0.10 | NIST Webbook |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C27893410&Units=SI

# 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

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|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |