

Benzene, (4-chlorobutyl)-

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| Other names: | (4-Chlorobutyl)benzene 1-Chloro-4-phenylbutane 4-Phenyl-n-butyl chloride 4-Phenylbutyl chloride |
| Inchi: | InChI=1S/C10H13Cl/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2 |
| InchiKey: | FLLZCZIHURYEQP-UHFFFAOYSA-N |
| Formula: | C10H13Cl |
| SMILES: | C1CCCCc1ccccc1 |
| Mol. weight [g/mol]: | 168.66 |
| CAS: | 4830-93-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 133.80 | kJ/mol | Joback Method |
| hf | -28.94 | kJ/mol | Joback Method |
| hfus | 19.89 | kJ/mol | Joback Method |
| hvap | 44.52 | kJ/mol | Joback Method |
| log10ws | -3.26 | | Crippen Method |
| logp | 3.248 | | Crippen Method |
| mcvol | 140.240 | ml/mol | McGowan Method |
| pc | 2817.33 | kPa | Joback Method |
| rinpol | 1256.00 | | NIST Webbook |
| tb | 492.31 | K | Joback Method |
| tc | 702.84 | K | Joback Method |
| tf | 258.80 | K | Joback Method |
| vc | 0.536 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 285.25 | J/molxK | 492.31 | Joback Method |
| cpg | 299.62 | J/molxK | 527.40 | Joback Method |
| cpg | 313.14 | J/molxK | 562.49 | Joback Method |
| cpg | 325.84 | J/molxK | 597.58 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 337.77 | J/molxK | 632.66 | Joback Method |
| cpg | 348.95 | J/molxK | 667.75 | Joback Method |
| cpg | 359.42 | J/molxK | 702.84 | Joback Method |
| dvisc | 0.0035067 | Paxs | 258.80 | Joback Method |
| dvisc | 0.0016801 | Paxs | 297.72 | Joback Method |
| dvisc | 0.0009542 | Paxs | 336.64 | Joback Method |
| dvisc | 0.0006094 | Paxs | 375.56 | Joback Method |
| dvisc | 0.0004234 | Paxs | 414.47 | Joback Method |
| dvisc | 0.0003131 | Paxs | 453.39 | Joback Method |
| dvisc | 0.0002429 | Paxs | 492.31 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.28852e+01 |
| Coeff. B | -3.58745e+03 |
| Coeff. C | -7.74460e+01 |
| Temperature range (K), min. | 362.22 |
| Temperature range (K), max. | 551.12 |

Sources

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|---|---|
| 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=C4830937&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|---------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |

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|------------------|---|
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| h vap: | 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 |
| pvap: | Vapor pressure |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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