

# Benzene, (4-chlorobutoxy)-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 1-Chloro-4-phenoxybutane<br>Ether, 4-chlorobutyl phenyl<br>4-Phenoxybutyl chloride<br>4-chlorobutyl phenyl ether |
| <b>Inchi:</b>               | InChI=1S/C10H13ClO/c11-8-4-5-9-12-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2  |
| <b>InchiKey:</b>            | JKXCPAVECBFBOC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C10H13ClO  |
| <b>SMILES:</b>              | C1CCCCOc1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 184.66   |
| <b>CAS:</b>                 | 2651-46-9  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 28.80   | kJ/mol               | Joback Method  |
| hf            | -161.16 | kJ/mol               | Joback Method  |
| hfus          | 21.08   | kJ/mol               | Joback Method  |
| hvap          | 46.93   | kJ/mol               | Joback Method  |
| log10ws       | -3.00   |                      | Crippen Method |
| logp          | 3.084   |                      | Crippen Method |
| mcvol         | 146.110 | ml/mol               | McGowan Method |
| pc            | 2767.17 | kPa                  | Joback Method  |
| tb            | 514.73  | K                    | Joback Method  |
| tc            | 723.31  | K                    | Joback Method  |
| tf            | 281.03  | K                    | Joback Method  |
| vc            | 0.554   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 309.44 | J/mol×K | 514.73          | Joback Method |
| cpg           | 371.96 | J/mol×K | 688.54          | Joback Method |
| cpg           | 360.90 | J/mol×K | 653.78          | Joback Method |
| cpg           | 349.13 | J/mol×K | 619.02          | Joback Method |
| cpg           | 336.65 | J/mol×K | 584.26          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 323.43    | J/molxK | 549.49 | Joback Method |
| cpg   | 382.34    | J/molxK | 723.31 | Joback Method |
| dvisc | 0.0002014 | Paxs    | 514.73 | Joback Method |
| dvisc | 0.0002589 | Paxs    | 475.78 | Joback Method |
| dvisc | 0.0003481 | Paxs    | 436.83 | Joback Method |
| dvisc | 0.0004958 | Paxs    | 397.88 | Joback Method |
| dvisc | 0.0007627 | Paxs    | 358.93 | Joback Method |
| dvisc | 0.0013029 | Paxs    | 319.98 | Joback Method |
| dvisc | 0.0025817 | Paxs    | 281.03 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 420.20 | K    | 1.60           | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2651469&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2651469&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvac:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mccol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |

|              |                                   |
|--------------|-----------------------------------|
| <b>tb:</b>   | Normal Boiling Point Temperature  |
| <b>tbrp:</b> | Boiling point at reduced pressure |
| <b>tc:</b>   | Critical Temperature              |
| <b>tf:</b>   | Normal melting (fusion) point     |
| <b>vc:</b>   | Critical Volume                   |

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