

Benzene, 1-chloro-4-(chloromethyl)-

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|-----------------------------|---|
| Other names: | (4-Chlorophenyl)methyl chloride 1-Chloro-4-(chloromethyl)benzene 4-Chlorobenzyl chloride NSC 34032 Toluene, p, «alpha»-dichloro- Toluene, p, «alpha»-dichloro- p, «alpha»-Dichlorotoluene p, «alpha»-Dichlorotoluene p-Chlorobenzyl chloride p-Chlorophenylmethyl chloride «alpha»,4-Dichlorotoluene «alpha»,p-Dichlorotoluene «alpha»,4-Dichlorotoluene «alpha»,p-Dichlorotoluene |
| Inchi: | InChI=1S/C7H6Cl2/c8-5-6-1-3-7(9)4-2-6/h1-4H,5H2 |
| InchiKey: | JQZAEUFPPSRDOP-UHFFFAOYSA-N |
| Formula: | C7H6Cl2 |
| SMILES: | ClCc1ccc(Cl)cc1 |
| Mol. weight [g/mol]: | 161.03 |
| CAS: | 104-83-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 86.98 | kJ/mol | Joback Method |
| hf | 5.77 | kJ/mol | Joback Method |
| hfus | 15.93 | kJ/mol | Joback Method |
| hvap | 42.88 | kJ/mol | Joback Method |
| log10ws | -3.19 | | Crippen Method |
| logp | 3.079 | | Crippen Method |
| mcvol | 110.210 | ml/mol | McGowan Method |
| pc | 3682.02 | kPa | Joback Method |
| tb | 466.08 | K | Joback Method |
| tc | 694.10 | K | Joback Method |
| tf | 267.43 | K | Joback Method |
| vc | 0.417 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 186.80 | J/molxK | 466.08 | Joback Method |
| cpg | 196.57 | J/molxK | 504.08 | Joback Method |
| cpg | 205.68 | J/molxK | 542.09 | Joback Method |
| cpg | 214.17 | J/molxK | 580.09 | Joback Method |
| cpg | 222.08 | J/molxK | 618.09 | Joback Method |
| cpg | 229.42 | J/molxK | 656.09 | Joback Method |
| cpg | 236.24 | J/molxK | 694.10 | Joback Method |
| dvisc | 0.0022622 | Paxs | 267.43 | Joback Method |
| dvisc | 0.0013273 | Paxs | 300.54 | Joback Method |
| dvisc | 0.0008657 | Paxs | 333.65 | Joback Method |
| dvisc | 0.0006099 | Paxs | 366.75 | Joback Method |
| dvisc | 0.0004554 | Paxs | 399.86 | Joback Method |
| dvisc | 0.0003555 | Paxs | 432.97 | Joback Method |
| dvisc | 0.0002875 | Paxs | 466.08 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.54460e+01 |
| Coeff. B | -4.32529e+03 |
| Coeff. C | -7.90800e+01 |
| Temperature range (K), min. | 364.42 |
| Temperature range (K), max. | 505.87 |

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=C104836&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>

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 |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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