# Benzene, 1,2,4,5-tetrachloro-3,6-bis(chloromethyl)-

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|---|---|
| **Other names:** | «alpha»,«alpha»',2,3,5,6-Hexachloro-p-xylene |
| | Tetrachloro-p-xylene dichloride |
| | p-Xylene, «alpha»,«alpha»',2,3,5,6-hexachloro- |
| | p-Tetrachloroxylylene dichloride |
| | 1,2,4,5-Tetrachloro-3,6-bis(chloromethyl)benzene |
| | 1,4-Bis(chloromethyl)tetrachlorobenzene |
| | alpha,alpha',2,3,5,6-hexachloro-4-xylene |
| **Inchi:** | InChI=1S/C8H4Cl6/c9-1-3-5(11)7(13)4(2-10)8(14)6(3)12/h1-2H2 |
| **InchiKey:** | IYGDLOMSJZQSGY-UHFFFAOYSA-N |
| **Formula:** | C8H4Cl6 |
| **SMILES:** | ClCc1c(Cl)c(Cl)c(CCl)c(Cl)c1Cl |
| **Mol. weight [g/mol]:** | 312.83 |
| **CAS:** | 1079-17-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 9.16 | kJ/mol | Joback Method |
| hf | -123.71 | kJ/mol | Joback Method |
| hfus | 33.75 | kJ/mol | Joback Method |
| hvap | 65.30 | kJ/mol | Joback Method |
| log10ws | -6.28 | | Crippen Method |
| logp | 5.778 | | Crippen Method |
| mcvol | 173.260 | ml/mol | McGowan Method |
| pc | 2624.46 | kPa | Joback Method |
| tb | 658.60 | K | Joback Method |
| tc | 903.12 | K | Joback Method |
| tf | 448.46 | K | Joback Method |
| vc | 0.669 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 304.03 | J/mol×K | 658.60 | Joback Method |
| cpg | 333.93 | J/mol×K | 862.37 | Joback Method |

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|---|---|---|---|---|
| cpg | 328.87 | J/mol×K | 821.61 | Joback Method |
| cpg | 323.37 | J/mol×K | 780.86 | Joback Method |
| cpg | 317.40 | J/mol×K | 740.11 | Joback Method |
| cpg | 310.96 | J/mol×K | 699.35 | Joback Method |
| cpg | 338.56 | J/mol×K | 903.12 | Joback Method |
| dvisc | 0.0002185 | Pa×s | 658.60 | Joback Method |
| dvisc | 0.0002562 | Pa×s | 623.58 | Joback Method |
| dvisc | 0.0003062 | Pa×s | 588.55 | Joback Method |
| dvisc | 0.0003744 | Pa×s | 553.53 | Joback Method |
| dvisc | 0.0004703 | Pa×s | 518.51 | Joback Method |
| dvisc | 0.0006106 | Pa×s | 483.48 | Joback Method |
| dvisc | 0.0008257 | Pa×s | 448.46 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 493.20 | K | 4.00 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1079170&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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