# Phthalide, 4,5,6,7-tetrachloro-

| | |
|---|---|
| **Other names:** | Bayer 96610 |
| | KF-32 |
| | Rabcide |
| | 4,5,6,7-Tetrachlorophthalide |
| | 4,5,6,7-Tetrachloro-2-benzofuran-1(3H)-one |
| | Fthalide |
| | Tetrachlorophthalide |
| | 1(3H)-Isobenzofuranone, 4,5,6,7-tetrachloro- |
| | phthalide |
| **Inchi:** | InChI=1S/C8H2Cl4O2/c9-4-2-1-14-8(13)3(2)5(10)7(12)6(4)11/h1H2 |
| **InchiKey:** | NMWKWBPNKPGATC-UHFFFAOYSA-N |
| **Formula:** | C8H2Cl4O2 |
| **SMILES:** | O=C1OCc2c(Cl)c(Cl)c(Cl)c(Cl)c21 |
| **Mol. weight [g/mol]:** | 271.91 |
| **CAS:** | 27355-22-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -107.23 | kJ/mol | Joback Method |
| hf | -268.79 | kJ/mol | Joback Method |
| hfus | 29.91 | kJ/mol | Joback Method |
| hvap | 65.51 | kJ/mol | Joback Method |
| log10ws | -4.81 | | Crippen Method |
| logp | 3.971 | | Crippen Method |
| mcvol | 145.360 | ml/mol | McGowan Method |
| pc | 3505.43 | kPa | Joback Method |
| rinpol | 2049.00 | | NIST Webbook |
| ripol | 3079.00 | | NIST Webbook |
| tb | 689.92 | K | Joback Method |
| tc | 954.43 | K | Joback Method |
| tf | 505.59 | K | Joback Method |
| vc | 0.557 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 283.00 | J/mol×K | 689.92 | Joback Method |
| cpg | 290.37 | J/mol×K | 734.00 | Joback Method |
| cpg | 297.17 | J/mol×K | 778.09 | Joback Method |
| cpg | 303.40 | J/mol×K | 822.17 | Joback Method |
| cpg | 309.09 | J/mol×K | 866.26 | Joback Method |
| cpg | 314.24 | J/mol×K | 910.34 | Joback Method |
| cpg | 318.88 | J/mol×K | 954.43 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C27355222&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
**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
**rinpol:** Non-polar retention indices
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume