# Sulphenone

| | |
|---|---|
| **Other names:** | Benzene, 1-chloro-4-(phenylsulfonyl)- |
| | Sulfone, p-chlorophenyl phenyl |
| | p-Chlorophenyl phenyl sulfone |
| | R 242 |
| | Sulfenon |
| | 4-Chlorodiphenyl sulfone |
| | 4-Chlorophenyl phenyl sulfone |
| | p-Monochlorophenyl phenyl sulfone |
| | R-242-B |
| | Compound R-242 |
| | ENT 17,941 |
| | Sulfenone |
| | Trifenson |
| | 4-Chlordifenylsulfon |
| | 4-Chlorodiphenyl sulphone |
| | p-Chlorophenyl phenyl sulphone |
| | 1-Chloro-4-(phenylsulfonyl)benzene |
| | NSC 404335 |
| **Inchi:** | InChI=1S/C12H9ClO2S/c13-10-6-8-12(9-7-10)16(14,15)11-4-2-1-3-5-11/h1-9H |
| **InchiKey:** | OFCFYWOKHPOXKF-UHFFFAOYSA-N |
| **Formula:** | C12H9ClO2S |
| **SMILES:** | O=S(=O)(c1ccccc1)c1ccc(Cl)cc1 |
| **Mol. weight [g/mol]:** | 252.72 |
| **CAS:** | 80-00-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -215.12 | kJ/mol | Joback Method |
| hf | -298.51 | kJ/mol | Joback Method |
| hfus | 30.10 | kJ/mol | Joback Method |
| hvap | 70.54 | kJ/mol | Joback Method |
| log10ws | -3.52 | | Crippen Method |
| logp | 3.173 | | Crippen Method |
| mcvol | 172.750 | ml/mol | McGowan Method |
| pc | 3881.95 | kPa | Joback Method |
| tb | 617.51 | K | Joback Method |
| tc | 860.39 | K | Joback Method |

| | | | |
|---|---|---|---|
| tf | 358.84 | K | Joback Method |
| vc | 0.666 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 385.19 | J/mol×K | 617.51 | Joback Method |
| cpg | 399.54 | J/mol×K | 657.99 | Joback Method |
| cpg | 412.66 | J/mol×K | 698.47 | Joback Method |
| cpg | 424.60 | J/mol×K | 738.95 | Joback Method |
| cpg | 435.39 | J/mol×K | 779.43 | Joback Method |
| cpg | 445.07 | J/mol×K | 819.91 | Joback Method |
| cpg | 453.69 | J/mol×K | 860.39 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C80002&Units=SI

# 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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume