# Benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]-

**Other names:** Sulfone, p-chlorophenyl 2,4,5-trichlorophenyl
p-Chlorophenyl 2,4,5-trichlorophenyl sulfone
Akaritox
Aredion
Duphar
Mition
Polacaritox
Roztoczol
Roztoczol extra
Tedion
Tedion V-18
Tetradiphon
V-18
2,4,4',5-Tetrachlorodiphenyl sulfone
4-Chlorophenyl 2,4,5-trichlorophenyl sulfone
p-Chlorophenyl 2,4,5-trichlorophenyl sulphone
ENT 23,737
FMC 5488
NIA 5488
Roztozol
Sulfone, 2,4,4',5-tetrachlorodiphenyl
2,4,4',5-Tetrachloor-difenyl-sulfon
3,4,6,4'-Tetrachlor-diphenylsulfon
2,4,4',5-Tetrachlor-diphenyl-sulfon
2,4,5,4'-Tetrachlorodiphenyl sulfone
2,4,5,4'-Tetrachlorodiphenylsulphone
2,4,4',5-Tetracloro-difenil-solfone
Tetradichlone
Tetrafidon
1,2,4-Trichloro-5-[(4-chlorophenyl)sulfonyl]benzene
Acaroil TD
Acarvin
Agrex T-7.5
Aracnol K
Mitifon
Tetradifon

**Inchi:** InChI=1S/C12H6Cl4O2S/c13-7-1-3-8(4-2-7)19(17,18)12-6-10(15)9(14)5-11(12)16/h1-6H

**InchiKey:** MLGCXEBRWGEOQX-UHFFFAOYSA-N

**Formula:** C12H6Cl4O2S

**SMILES:** O=S(=O)(c1ccc(Cl)cc1)c1cc(Cl)c(Cl)cc1Cl

**Mol. weight [g/mol]:** 356.05
**CAS:** 116-29-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -279.80 | kJ/mol | Joback Method |
| hf | -380.14 | kJ/mol | Joback Method |
| hfus | 41.53 | kJ/mol | Joback Method |
| hvap | 85.68 | kJ/mol | Joback Method |
| log10ws | -5.58 | | Crippen Method |
| logp | 5.133 | | Crippen Method |
| mcvol | 209.470 | ml/mol | McGowan Method |
| pc | 3224.64 | kPa | Joback Method |
| rinpol | 2533.00 | | NIST Webbook |
| rinpol | 2462.00 | | NIST Webbook |
| rinpol | 2536.00 | | NIST Webbook |
| rinpol | 2522.00 | | NIST Webbook |
| rinpol | 2536.00 | | NIST Webbook |
| rinpol | 2533.00 | | NIST Webbook |
| rinpol | 2522.00 | | NIST Webbook |
| rinpol | 2462.00 | | NIST Webbook |
| tb | 744.74 | K | Joback Method |
| tc | 997.53 | K | Joback Method |
| tf | 420.09 ± 0.20 | K | NIST Webbook |
| tf | 420.10 ± 0.20 | K | NIST Webbook |
| vc | 0.814 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 447.94 | J/mol×K | 744.74 | Joback Method |
| cpg | 457.81 | J/mol×K | 786.87 | Joback Method |
| cpg | 466.58 | J/mol×K | 829.00 | Joback Method |
| cpg | 474.30 | J/mol×K | 871.14 | Joback Method |
| cpg | 480.96 | J/mol×K | 913.27 | Joback Method |
| cpg | 486.62 | J/mol×K | 955.40 | Joback Method |
| cpg | 491.28 | J/mol×K | 997.53 | Joback Method |

| | | | | |
|---|---|---|---|---|
| hfust | 28.94 | kJ/mol | 419.90 | NIST Webbook |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116290&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 |

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |