# P-phenylenediamine, n,n-dimethyl, n',n'-bis(p-tolylsulfonyl)-

**Inchi:** InChI=1S/C22H24N2O4S2/c1-17-5-13-21(14-6-17)29(25,26)24(20-11-9-19(10-12-20)23(

**InchiKey:** CXIBFOYRMRNMRY-UHFFFAOYSA-N

**Formula:** C22H24N2O4S2

**SMILES:** Cc1ccc(S(=O)(=O)N(c2ccc(N(C)C)cc2)S(=O)(=O)c2ccc(C)cc2)cc1

**Mol. weight [g/mol]:** 444.57

**CAS:** 19770-85-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -272.82 | kJ/mol | Joback Method |
| hf | -593.87 | kJ/mol | Joback Method |
| hfus | 62.49 | kJ/mol | Joback Method |
| hvap | 114.74 | kJ/mol | Joback Method |
| log10ws | -5.23 | | Crippen Method |
| logp | 3.954 | | Crippen Method |
| mcvol | 325.700 | ml/mol | McGowan Method |
| pc | 2320.31 | kPa | Joback Method |
| tb | 918.18 | K | Joback Method |
| tc | 1146.79 | K | Joback Method |
| tf | 596.58 | K | Joback Method |
| vc | 1.232 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 977.64 | J/mol×K | 918.18 | Joback Method |
| cpg | 990.95 | J/mol×K | 956.28 | Joback Method |
| cpg | 1002.58 | J/mol×K | 994.38 | Joback Method |
| cpg | 1012.57 | J/mol×K | 1032.49 | Joback Method |
| cpg | 1021.00 | J/mol×K | 1070.59 | Joback Method |
| cpg | 1027.94 | J/mol×K | 1108.69 | Joback Method |
| cpg | 1033.46 | J/mol×K | 1146.79 | 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=C19770855&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 |