# P-toluenesulfonamide, n,n'-(1,4-cyclohexylene)bis[n-(2-hydroxyethyl)-, diacetate

**Inchi:** InChI=1S/C28H38N2O8S2/c1-21-5-13-27(14-6-21)39(33,34)29(17-19-37-23(3)31)25-9-1

**InchiKey:** VENNTHBQQAJMQS-UHFFFAOYSA-N

**Formula:** C28H38N2O8S2

**SMILES:** CC(=O)OCCN(C1CCC(N(CCOC(C)=O)S(=O)(=O)c2ccc(C)cc2)CC1)S(=O)(=O)c1ccc(C)c

**Mol. weight [g/mol]:** 594.74

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -776.18 | kJ/mol | Joback Method |
| hf | -1398.39 | kJ/mol | Joback Method |
| hfus | 82.86 | kJ/mol | Joback Method |
| hvap | 143.59 | kJ/mol | Joback Method |
| log10ws | -5.45 | | Crippen Method |
| logp | 3.422 | | Crippen Method |
| mcvol | 438.020 | ml/mol | McGowan Method |
| pc | 1367.69 | kPa | Joback Method |
| tb | 1191.26 | K | Joback Method |
| tc | 1465.13 | K | Joback Method |
| tf | 772.72 | K | Joback Method |
| vc | 1.655 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1489.00 | J/mol×K | 1191.26 | Joback Method |
| cpg | 1490.92 | J/mol×K | 1236.91 | Joback Method |
| cpg | 1489.42 | J/mol×K | 1282.55 | Joback Method |
| cpg | 1484.56 | J/mol×K | 1328.20 | Joback Method |
| cpg | 1476.41 | J/mol×K | 1373.84 | Joback Method |
| cpg | 1465.05 | J/mol×K | 1419.49 | Joback Method |
| cpg | 1450.55 | J/mol×K | 1465.13 | 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=B6007362&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 |