# 4-Toluenesulfonic acid 4-azulylethyl ester

**Inchi:** InChI=1S/C19H18O3S/c1-15-9-11-18(12-10-15)23(20,21)22-14-13-17-6-3-2-5-16-7-4-8-1
**InchiKey:** INMMWFDWWQDEBX-UHFFFAOYSA-N
**Formula:** C19H18O3S
**SMILES:** Cc1ccc(S(=O)(=O)OCCc2ccccc3cccc2-3)cc1
**Mol. weight [g/mol]:** 326.41
**CAS:** 26154-63-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -152.23 | kJ/mol | Joback Method |
| hf | -379.87 | kJ/mol | Joback Method |
| hfus | 41.85 | kJ/mol | Joback Method |
| hvap | 86.45 | kJ/mol | Joback Method |
| ie | 7.30 | eV | NIST Webbook |
| log10ws | -5.77 | | Crippen Method |
| logp | 4.048 | | Crippen Method |
| mcvol | 245.550 | ml/mol | McGowan Method |
| pc | 2433.84 | kPa | Joback Method |
| tb | 786.62 | K | Joback Method |
| tc | 1018.90 | K | Joback Method |
| tf | 475.26 | K | Joback Method |
| vc | 0.950 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 684.04 | J/mol×K | 786.62 | Joback Method |
| cpg | 699.52 | J/mol×K | 825.33 | Joback Method |
| cpg | 713.65 | J/mol×K | 864.05 | Joback Method |
| cpg | 726.48 | J/mol×K | 902.76 | Joback Method |
| cpg | 738.06 | J/mol×K | 941.47 | Joback Method |
| cpg | 748.48 | J/mol×K | 980.18 | Joback Method |
| cpg | 757.78 | J/mol×K | 1018.90 | Joback Method |

# Sources

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|---|---|
| **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=C26154632&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **ie:** | Ionization energy |
| **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 |