

# p-Toluenesulfonamide, alpha-9H-adenin-9-yl-

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | «alpha»-[6-Amino-9H-purin-9-yl]-p-toluenesulfonamide                             |
| Inchi:               | InChI=1S/C12H12N6O2S/c13-11-10-12(16-6-15-11)18(7-17-10)5-8-1-3-9(4-2-8)21(14,19 |
| InchiKey:            | HYXXGPTXYDTSMD-UHFFFAOYSA-N                                                      |
| Formula:             | C12H12N6O2S                                                                      |
| SMILES:              | Nc1ncnc2c1ncn2Cc1ccc(S(N)(=O)=O)cc1                                              |
| Mol. weight [g/mol]: | 304.33                                                                           |
| CAS:                 | 21267-98-1                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.47   |        | Crippen Method |
| logp          | 0.104   |        | Crippen Method |
| mcvol         | 205.230 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21267981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21267981&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                             |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |

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