

# N4-Acetyl sulfameter

**Inchi:** InChI=1S/C13H14N4O4S/c1-9(18)16-10-3-5-12(6-4-10)22(19,20)17-13-14-7-11(21-2)8-1  
**InchiKey:** GUKOCAZFTOVPIIS-UHFFFAOYSA-N  
**Formula:** C13H14N4O4S  
**SMILES:** COc1cnc(NS(=O)(=O)c2ccc(NC(C)=O)cc2)nc1  
**Mol. weight [g/mol]:** 322.34

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.83   |        | Crippen Method |
| logp          | 1.244   |        | Crippen Method |
| mcvol         | 221.960 | ml/mol | McGowan Method |
| rinpol        | 3090.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525585&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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