# Trimethylsilyl 3-(aminosulfonyl)-5-[butyl(trimethylsilyl)amino]-4-

**Other names:** Bumetanide, 2tms derivative

**Inchi:** InChI=1S/C23H36N2O5SSi2/c1-8-9-15-25(32(2,3)4)20-16-18(23(26)30-33(5,6)7)17-21(3

**InchiKey:** WQPNCSWEDODDPM-UHFFFAOYSA-N

**Formula:** C23H36N2O5SSi2

**SMILES:** CCCCN(c1cc(C(=O)O[Si](C)(C)C)cc(S(N)(=O)=O)c1Oc1ccccc1)[Si](C)(C)C

**Mol. weight [g/mol]:** 508.78

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.99 | | Crippen Method |
| logp | 5.559 | | Crippen Method |
| rinpol | 3032.50 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U333190&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices