

3-tert-Butyldimethylsilylamino-1,2,4-triazole

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|----------------------|---|
| Other names: | 3-Amino-2H-1,2,4-triazole BDMS |
| Inchi: | InChI=1S/C8H18N4Si/c1-8(2,3)13(4,5)12-7-9-6-10-11-7/h6H,1-5H3,(H2,9,10,11,12) |
| InchiKey: | SLQKHYQPUCCB-UHFFFAOYSA-N |
| Formula: | C8H18N4Si |
| SMILES: | CC(C)(C)[Si](C)(C)Nc1ncn[nH]1 |
| Mol. weight [g/mol]: | 198.34 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.37 | | Crippen Method |
| logp | 1.740 | | Crippen Method |
| rinpol | 1451.00 | | NIST Webbook |
| rinpol | 1451.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373054&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 |
| rinpol: | Non-polar retention indices |

Latest version available from:

<https://www.chemeo.com/cid/65-133-2/3-tert-Butyldimethylsilylamino-1-2-4-triazole.pdf>

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