

# 4-Cyano-1-dimethyl(tert-butyl)silyloxybenzene

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 4-Cyanophenol, tbdms derivative  |
| <b>Inchi:</b>               | InChI=1S/C13H19NOSi/c1-13(2,3)16(4,5)15-12-8-6-11(10-14)7-9-12/h6-9H,1-5H3 |
| <b>InchiKey:</b>            | FFJFJEYUUBQRSB-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C13H19NOSi   |
| <b>SMILES:</b>              | CC(C)(C)[Si](C)(C)Oc1ccc(C#N)cc1   |
| <b>Mol. weight [g/mol]:</b> | 233.38   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.09   |      | Crippen Method |
| logp          | 3.942   |      | Crippen Method |
| rinpola       | 1597.00 |      | NIST Webbook   |
| rinpola       | 1597.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307923&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307923&amp;Units=SI</a> |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>rinpola:</b> | Non-polar retention indices         |

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