

# 2-Chloro-4-fluoro-phenol, tert-butyldimethylsilyl ether

|                      |                                                                                                                                          |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Chloro-4-fluorophenol t-butyldimethylsilyl ether<br>Phenol, 2-chloro-4-fluoro-O-t-butyldimethylsilyl-<br>2-Chloro-4-fluoro-phenol BDMS |
| Inchi:               | InChI=1S/C12H18ClFOSi/c1-12(2,3)16(4,5)15-11-7-6-9(14)8-10(11)13/h6-8H,1-5H3                                                             |
| InchiKey:            | OQLJQUCHSRMIPC-UHFFFAOYSA-N                                                                                                              |
| Formula:             | C12H18ClFOSi                                                                                                                             |
| SMILES:              | CC(C)(C)[Si](C)(C)Oc1ccc(F)cc1Cl                                                                                                         |
| Mol. weight [g/mol]: | 260.81                                                                                                                                   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.75   |      | Crippen Method |
| logp          | 4.863   |      | Crippen Method |
| rinpol        | 1433.00 |      | NIST Webbook   |
| rinpol        | 1433.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373405&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 |
| rinpol:  | Non-polar retention indices         |

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