

Isopropyl 2-[4-(tert-butyl dimethylsilyl)oxyphenyl]acetate

Other names: 4-Hydroxyphenylacetic acid, isopropyl ester, t-butyl dimethylsilyl
Inchi: InChI=1S/C16H26O3Si/c1-12(2)18-15(17)13-8-10-14(11-9-13)19-20(6,7)16(3,4)5/h8-12H
InchiKey: VAWVHTGKCLAKTE-UHFFFAOYSA-N
Formula: C16H26O3Si
SMILES: CC(C)OC(=O)c1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 294.46

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.93 | | Crippen Method |
| logp | 4.636 | | Crippen Method |
| rinpol | 1858.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373378&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

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