

Trimethylsilyl 2-amino-3-(3-chloro-4-[(trimethylsilyl)oxy]phenyl)propanoate

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| Other names: | 2-Amino-3-(3-chloro-4-hydroxy-phenyl)propanoic acid, O, O'-bis(trimethylsilyl)- Trimethylsilyl 2-amino-3-(3-chloro-4-[(trimethylsilyl)oxy]phenyl)propanoate |
| Inchi: | InChI=1S/C15H26ClNO3Si2/c1-21(2,3)19-14-8-7-11(9-12(14)16)10-13(17)15(18)20-22(4) |
| InchiKey: | HOUWOLDVTDFTBV-UHFFFAOYSA-N |
| Formula: | C15H26ClNO3Si2 |
| SMILES: | <chem>C[Si](C)(C)OC(=O)C(N)Cc1ccc(O[Si](C)(C)C)c(Cl)c1</chem> |
| Mol. weight [g/mol]: | 360.00 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.10 | | Crippen Method |
| logp | 3.802 | | Crippen Method |
| rinpol | 2062.00 | | NIST Webbook |
| rinpol | 2062.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U378756&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

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