

(2-Bromophenyl)methanol, dimethylpentafluorophenylsilyl ether

Inchi: InChI=1S/C15H12BrF5OSi/c1-23(2,22-7-8-5-3-4-6-9(8)16)15-13(20)11(18)10(17)12(19)1
InchiKey: BKJFRXNKENQHQO-UHFFFAOYSA-N
Formula: C15H12BrF5OSi
SMILES: C[Si](C)(OCc1ccccc1Br)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 411.24

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -8.74 | | Crippen Method |
| logp | 4.774 | | Crippen Method |
| rinpol | 1882.00 | | NIST Webbook |
| rinpol | 1882.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368716&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/118-331-3/2-Bromophenyl-methanol-dimethylpentafluorophenylsilyl-ether.pdf>

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