

Benzoic acid, 4-heptafluorobutyrylthio-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F7O3SSi/c1-26(2,3)24-10(22)8-4-6-9(7-5-8)25-11(23)12(15,16)13(17,18)14
InchiKey: GUCQJYHZEGZCRP-UHFFFAOYSA-N
Formula: C14H13F7O3SSi
SMILES: C[Si](C)(C)OC(=O)c1ccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 422.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	5.130		Crippen Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375185&Units=SI>

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/114-817-8/Benzoic-acid-4-heptafluorobutyrylthio-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-03 18:47:41.490272722 +0000 UTC m=+17051310.410850033.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.