

Benzeneacetic acid, «alpha»-methyl-4-(2-methylpropyl)-, trimethylsilyl ester

Other names:

Monotrimethylsilyl derivative of Ibuprofen

Inchi: InChI=1S/C16H26O2Si/c1-12(2)11-14-7-9-15(10-8-14)13(3)16(17)18-19(4,5)6/h7-10,12-

InchiKey: YCAAUQGUAZTIAV-UHFFFAOYSA-N

Formula: C16H26O2Si

SMILES: CC(C)Cc1ccc(C(C)C(=O)O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 278.46

CAS: 74810-89-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	4.367		Crippen Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C74810892&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

Latest version available from:

<https://www.chemeo.com/cid/113-940-2/Benzeneacetic-acid-alpha-methyl-4-2-methylpropyl-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-02 23:52:08.56275949 +0000 UTC m=+16983177.483336805.

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