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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient