

Benzoic acid, 3-acetylthio-, trimethylsilyl ester

Inchi:	InChI=1S/C12H16O3SSi/c1-9(13)16-11-7-5-6-10(8-11)12(14)15-17(2,3)4/h5-8H,1-4H3
InchiKey:	NJLWCBFCICHNCF-UHFFFAOYSA-N
Formula:	C12H16O3SSi
SMILES:	CC(=O)Sc1cccc(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]:	268.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	3.317		Crippen Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		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=U375177&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/122-766-6/Benzoic-acid-3-acetylthio-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-28 04:12:27.111368309 +0000 UTC m=+16566796.031945625.

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