

3-Indoleacetic acid, trimethylsilyl ester

Other names:	3-Indoleacetic acid, TMS 3-Indoleacetic acid, tms derivative
Inchi:	InChI=1S/C13H17NO2Si/c1-17(2,3)16-13(15)8-10-9-14-12-7-5-4-6-11(10)12/h4-7,9,14H
InchiKey:	PNYNSYZOBWBNFR-UHFFFAOYSA-N
Formula:	C13H17NO2Si
SMILES:	C[Si](C)(C)OC(=O)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	247.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	2.607		Crippen Method
rinpola	1941.20		NIST Webbook
rinpola	1941.20		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333672&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/118-743-6/3-Indoleacetic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-01 03:03:10.113199249 +0000 UTC m=+16821839.033776564.

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