

Niflumic acid tbdms

Other names:	Niflumic acid, tbdms derivative
Inchi:	InChI=1S/C19H23F3N2O2Si/c1-18(2,3)27(4,5)26-17(25)15-10-7-11-23-16(15)24-14-9-6
InchiKey:	ABVMYTKMQZELRT-UHFFFAOYSA-N
Formula:	C19H23F3N2O2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1cccnc1Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	396.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	6.006		Crippen Method
rinsol	2335.60		NIST Webbook
rinsol	2335.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U331798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/47-436-6/Niflumic-acid-tbdms.pdf>

Generated by Cheméo on 2024-04-28 10:52:59.875211941 +0000 UTC m=+16590828.795789259.

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