

N-Desmethylflunitrazepam, trimethylsilyl derivative

Inchi:	InChI=1S/C18H18FN3O3Si/c1-26(2,3)25-17-11-20-18(13-6-4-5-7-15(13)19)14-10-12(22)
InchiKey:	WJKWHPXTZPEKFR-UHFFFAOYSA-N
Formula:	C18H18FN3O3Si
SMILES:	C[Si](C)(C)OC1=Nc2ccc([N+](=O)[O-])cc2C(c2ccccc2F)=NC1
Mol. weight [g/mol]:	371.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	4.466		Crippen Method
rinpol	2538.60		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U417192&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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/81-751-8/N-Desmethylflunitrazepam-trimethylsilyl-derivative.pdf>

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