

3-O-methyl dopamine, PFB-TMS

Inchi: InChI=1S/C19H20F5NO3Si/c1-27-12-9-10(5-6-11(12)28-29(2,3)4)7-8-25-19(26)13-14(20)
InchiKey: LMCZYNQIPQCNAP-UHFFFAOYSA-N
Formula: C19H20F5NO3Si
SMILES: COc1cc(CCN(C=O)c2c(F)c(F)c(F)c(F)c2F)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 433.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.577		Crippen Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		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=R305752&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/60-742-1/3-O-methyl-dopamine-PFB-TMS.pdf>

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