

Dopamine, PFB-TMS

Inchi: InChI=1S/C21H26F5NO3Si2/c1-31(2,3)29-13-8-7-12(11-14(13)30-32(4,5)6)9-10-27-21(2)
InchiKey: FMPNZWUCJCQBJZ-UHFFFAOYSA-N
Formula: C21H26F5NO3Si2
SMILES: C[Si](C)(C)Oc1ccc(CCNC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 491.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	5.782		Crippen Method
rinpol	2184.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R305767&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/17-339-7/Dopamine-PFB-TMS.pdf>

Generated by Cheméo on 2024-04-17 02:55:15.361234108 +0000 UTC m=+15611764.281811424.

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