

N-(trifluoroacetyl)-o,o',o''-tris(trimethylsilyl)norepinephrine

Other names:	Noradrenaline, N-TFA-O-TMS
Inchi:	InChI=1S/C19H34F3NO4Si3/c1-28(2,3)25-15-11-10-14(12-16(15)26-29(4,5)6)17(27-30(7
InchiKey:	CRFVINPEQAEMIM-UHFFFAOYSA-N
Formula:	C19H34F3NO4Si3
SMILES:	C[Si](C)(C)Oc1ccc(C(CNC(=O)C(F)(F)F)O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	481.74

Physical Properties

Property code	Value	Unit	Source
logp	5.685		Crippen Method
rinpol	1933.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U72263&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/28-047-9/N-trifluoroacetyl-o-o-o-tris-trimethylsilyl-norepinephrine.pdf>

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