

Normetanephryne, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C26H49NO5Si2/c1-19(2)18-30-24(28)27-17-23(32-34(12,13)26(6,7)8)20-14-15
InchiKey: SQUSOXBGPFWEBFD-UHFFFAOYSA-N
Formula: C26H49NO5Si2
SMILES: COc1cc(C(CNC(=O)OCC(C)C)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 511.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	7.524		Crippen Method
rinpol	2901.00		NIST Webbook
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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=R392786&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/12-298-8/Normetanephryne-N-isoBOC-O-TBDMS.pdf>

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