

Carazolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C27H38N2O6Si/c1-8-32-26(30)28(19(3)4)17-20(35-36(5,6)7)18-34-24-16-12-1
InchiKey: GTOGLBDDZXXJHK-UHFFFAOYSA-N
Formula: C27H38N2O6Si
SMILES: CCOC(=O)N(CC(COc1cccc2c1c1ccccc1n2C(=O)OCC)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 514.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.70		Crippen Method
logp	6.265		Crippen Method
rinpol	3178.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435195&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/64-638-3/Carazolol-N-ethoxycarbonylated-TMS.pdf>

Generated by Cheméo on 2024-04-28 23:40:30.141339039 +0000 UTC m=+16636879.061916354.

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