

Desmethyldoxepin, N-trimethylsilyl-

Inchi: InChI=1S/C21H27NOSi/c1-22(24(2,3)4)15-9-13-19-18-11-6-5-10-17(18)16-23-21-14-8-7
InchiKey: FSKYDGSNDYHCAJ-UYRXBGFRSA-N
Formula: C21H27NOSi
SMILES: CN(CCC=C1c2ccccc2COc2ccccc21)[Si](C)(C)C
Mol. weight [g/mol]: 337.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	5.167		Crippen Method
rinpol	2424.60		NIST Webbook
rinpol	2424.60		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=U417185&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/96-261-6/Desmethyldoxepin-N-trimethylsilyl.pdf>

Generated by Cheméo on 2024-04-28 15:43:45.065497343 +0000 UTC m=+16608273.986074658.

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