

(-)-Isolongifolol, (3-cyanopropyl)dimethylsilyl ether

Inchi: InChI=1S/C21H37NOSi/c1-20(2)11-8-12-21(3)17-10-9-16(19(17)20)18(21)15-23-24(4,5)
InchiKey: JYXMBCXNZBDUBI-UHFFFAOYSA-N
Formula: C21H37NOSi
SMILES: CC1(C)CCCC2(C)C(CO[Si](C)(C)CCCC#N)C3CCC2C31
Mol. weight [g/mol]: 347.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	6.000		Crippen Method
rinpol	2341.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376206&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/53-016-5/Isolongifolol-3-cyanopropyl-dimethylsilyl-ether.pdf>

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