

Diethanolamine, N-isoBOC, O-TBDMS, # 1

Inchi: InChI=1S/C21H47NO4Si2/c1-18(2)17-24-19(23)22(13-15-25-27(9,10)20(3,4)5)14-16-26-
InchiKey: LLQVEJVRRLNCCK-UHFFFAOYSA-N
Formula: C21H47NO4Si2
SMILES: CC(C)COC(=O)N(CCO[Si](C)(C)C(C)(C)C)CCO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 433.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	6.125		Crippen Method
rinpol	2168.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R392424&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/66-431-0/Diethanolamine-N-isoBOC-O-TBDMS-1.pdf>

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