

bis O-TBDMS derivative of N-isoBOC diethanolamine

Other names:	Diethanolamine, N-isoBOC, O-TBDMS, # 2
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
rinsol	2284.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

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<https://www.cheméo.com/cid/120-208-7/bis-O-TBDMS-derivative-of-N-isoBOC-diethanolamine.pdf>

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