

2-Bromo-2-nitro-propane-1,3-diol, bis(trimethylsilyl)- ether

Inchi:	InChI=1S/C9H22BrNO4Si2/c1-16(2,3)14-7-9(10,11(12)13)8-15-17(4,5)6/h7-8H2,1-6H3
InchiKey:	UYQYBAFSNDXBNP-UHFFFAOYSA-N
Formula:	C9H22BrNO4Si2
SMILES:	C[Si](C)(C)OCC(Br)(CO[Si](C)(C)C)[N+](=O)[O-]
Mol. weight [g/mol]:	344.35

Physical Properties

Property code	Value	Unit	Source
log10ws	1.01		Crippen Method
logp	3.057		Crippen Method
rinpol	1439.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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