

Cytosine, 5-bromo-N,O-bis(trimethylsilyl)-

Other names:	5-Bromocytosine, di-TMS Cytosine, 5-bromo, N,O-bis-TMS Pyrimidine, 4-amino-2-hydroxy-5-bromo, bis-TMS Cytosine, 5-bromo, TMS 5-Bromocytosine, TMS Pyrimidine, 4-amino-2-hydroxy-5-bromo, TMS
Inchi:	InChI=1S/C10H20BrN3OSi2/c1-16(2,3)14-9-8(11)7-12-10(13-9)15-17(4,5)6/h7H,1-6H3,(
InchiKey:	FACYSDZVGGOMDR-UHFFFAOYSA-N
Formula:	C10H20BrN3OSi2
SMILES:	C[Si](C)(C)Nc1nc(O[Si](C)(C)C)ncc1Br
Mol. weight [g/mol]:	334.36
CAS:	50271-92-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.07		Crippen Method
logp	3.700		Crippen Method
rinpol	1615.60		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1615.60		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=C50271926&Units=SI

Legend

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

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