

5-Bromo-2,4-bis[(trimethylsilyl)oxy]pyrimidine

Other names:	Uracil, 5-bromo, TMS 5-Bromouracil, TMS
Inchi:	InChI=1S/C10H19BrN2O2Si2/c1-16(2,3)14-9-8(11)7-12-10(13-9)15-17(4,5)6/h7H,1-6H3
InchiKey:	YKWXYMHPDZTFOY-UHFFFAOYSA-N
Formula:	C10H19BrN2O2Si2
SMILES:	C[Si](C)(C)Oc1ncc(Br)c(O[Si](C)(C)C)n1
Mol. weight [g/mol]:	335.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.18		Crippen Method
logp	3.666		Crippen Method
rinpol	1529.10		NIST Webbook
rinpol	1529.10		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1531.20		NIST Webbook
rinpol	1531.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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