

Trimethylsilyl 3-(aminosulfonyl)-5-[butyl(trimethylsilyl)amino]-4-

Other names:	Bumetanide, 2tms derivative
Inchi:	InChI=1S/C23H36N2O5SSi2/c1-8-9-15-25(32(2,3)4)20-16-18(23(26)30-33(5,6)7)17-21(3
InchiKey:	WQPNCSEWEDODDPM-UHFFFAOYSA-N
Formula:	C23H36N2O5SSi2
SMILES:	CCCCN(c1cc(C(=O)O[Si](C)(C)C)cc(S(N)(=O)=O)c1Oc1ccccc1)[Si](C)(C)C
Mol. weight [g/mol]:	508.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	5.559		Crippen Method
rinpol	3032.50		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333190&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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