Trimethylsilyl 3-(aminosulfonyl)-5-(butylamino)-4-phenoxybenzo

Other names: Bumetanide, tms derivative
Inchi: InChI=1S/C20H28N2O5SSi/c1-5-6-12-22-17-13-15(20(23)27-29(2,3)4)14-18(28(21,24)25
InchiKey: SKGQFYOTNUIMGW-UHFFFAOYSA-N
Formula: C20H28N2O5SSi
SMILES: CCCCNc1cc(C(=O)O[Si](C)(C)C)cc(S(N)(=O)=O)c1Oc1ccccc1
Mol. weight [g/mol]: 436.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	4.330		Crippen Method
rinpol	3157.80		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333191&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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