

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

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)29)20
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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/50-803-4/Trimethylsilyl-3-aminosulfonyl-5-butylamino-4-phenoxybenzoate.pdf>

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