

3-Aminobenzoic acid, N- trifluoroacetyl -, N,O-bis(tert.-butyldimethylsilyl)-

Inchi: InChI=1S/C21H34F3NO3Si2/c1-19(2,3)29(7,8)25(18(27)21(22,23)24)16-13-11-12-15(14)
InchiKey: HICMNIMTZYKFGH-UHFFFAOYSA-N
Formula: C21H34F3NO3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(N(C(=O)C(F)(F)F)[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 461.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	6.749		Crippen Method
rinpol	2075.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375084&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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<https://www.chemeo.com/cid/69-310-1/3-Aminobenzoic-acid-N-trifluoroacetyl-N-O-bis-tert-butyldimethylsilyl.pdf>

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