

tert-Butyldimethylsilyl trifluoromethanesulfonate

Other names:	t-Butyldimethylsilyl triflate t-Butyldimethylsilyltrifluoromethanesulfonate Methanesulfonic acid, trifluoro-, (1,1-dimethylethyl)dimethylsilyl ester t-Butylmethylsilyl triflate tert-butyldimethylsilyl trifluoromethanesulphonate
Inchi:	InChI=1S/C7H15F3O3SSi/c1-6(2,3)15(4,5)13-14(11,12)7(8,9)10/h1-5H3
InchiKey:	WLLIXJBWWFGEHT-UHFFFAOYSA-N
Formula:	C7H15F3O3SSi
SMILES:	CC(C)(C)[Si](C)(C)OS(=O)(=O)C(F)(F)F
Mol. weight [g/mol]:	264.34
CAS:	69739-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Crippen Method
logp	2.858		Crippen Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.00 ± 1.00	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69739340&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
tbrp:	Boiling point at reduced pressure

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