

Bis(trimethylsilyl) sulfate

Other names:	Sulfuric acid, bis(trimethylsilyl) ester Silanol, trimethyl-, sulfate (2:1) Sulfuric acid, bis(trimethylsilyl)- Sulfuric acid, TMS bis(trimethylsilyl) sulphate
Inchi:	InChI=1S/C6H18O4SSi2/c1-12(2,3)9-11(7,8)10-13(4,5)6/h1-6H3
InchiKey:	KRUQDZRWZXUUAD-UHFFFAOYSA-N
Formula:	C6H18O4SSi2
SMILES:	C[Si](C)(C)OS(=O)(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	242.44
CAS:	18306-29-1

Physical Properties

Property code	Value	Unit	Source
log10ws	2.58		Crippen Method
logp	1.934		Crippen Method
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
tf	330.00 ± 1.00	K	NIST Webbook
tf	318.50 ± 0.50	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.00	K	2.40	NIST Webbook
tbrp	363.00	K	0.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18306291&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
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/72-998-5/Bis-trimethylsilyl-sulfate.pdf>

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