

1,2-Benzenedimethanethiol, S-trimethylsilyl-

Other names:	1,2-Benzenedimethanethiol, tms derivative
Inchi:	InChI=1S/C11H18S2Si/c1-14(2,3)13-9-11-7-5-4-6-10(11)8-12/h4-7,12H,8-9H2,1-3H3
InchiKey:	UOCQOJYGXKUJPM-UHFFFAOYSA-N
Formula:	C11H18S2Si
SMILES:	C[Si](C)(C)SCc1ccccc1CS
Mol. weight [g/mol]:	242.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	4.184		Crippen Method
rinpol	1985.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353029&Units=SI

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/78-858-4/1-2-Benzenedimethanethiol-S-trimethylsilyl.pdf>

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