

O-methylated salsolinol, TMS

Inchi: InChI=1S/C15H25NO2Si/c1-11-13-10-15(18-3)14(17-2)9-12(13)7-8-16(11)19(4,5)6/h9-1
InchiKey: WPMSYANNIBSIKO-NSHDSACASA-N
Formula: C15H25NO2Si
SMILES: COc1cc2c(cc1OC)C(C)N([Si](C)(C)C)CC2
Mol. weight [g/mol]: 279.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	3.458		Crippen Method
rinpol	1910.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R305069&Units=SI>

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.cheméo.com/cid/20-787-6/O-methylated-salsolinol-TMS.pdf>

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