

Phenol, 2-chloro-5-methoxy, TMS

Inchi: InChI=1S/C10H15ClO2Si/c1-12-8-5-6-9(11)10(7-8)13-14(2,3)4/h5-7H,1-4H3
InchiKey: JRIABOBTPFEUIC-UHFFFAOYSA-N
Formula: C10H15ClO2Si
SMILES: COc1ccc(Cl)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 230.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	3.562		Crippen Method
rinpol	1410.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R100488&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/50-786-4/Phenol-2-chloro-5-methoxy-TMS.pdf>

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