

Coniferyl aldehyde, trimethylsilyl ether

Inchi: InChI=1S/C13H18O3Si/c1-15-13-10-11(6-5-9-14)7-8-12(13)16-17(2,3)4/h5-10H,1-4H3/b
InchiKey: QVPSJMTZAAPWKX-AATRIKPKSA-N
Formula: C13H18O3Si
SMILES: COc1cc(C=CC=O)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 250.37
CAS: 130878-30-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	3.121		Crippen Method
rinpol	1852.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C130878307&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

Latest version available from:

<https://www.chemeo.com/cid/122-659-5/Coniferyl-aldehyde-trimethylsilyl-ether.pdf>

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