

oximated 4-hydroxyphenylpyruvic acid, diTMS

Inchi: InChI=1S/C15H25NO4Si2/c1-21(2,3)19-13-9-7-12(8-10-13)11-14(16-18)15(17)20-22(4,5)
InchiKey: MASKMSAKPKGSIN-PEZBUJJGSA-N
Formula: C15H25NO4Si2
SMILES: C[Si](C)(C)OC(=O)C(Cc1ccc(O[Si](C)(C)C)cc1)=NO
Mol. weight [g/mol]: 339.53

Physical Properties

Property code	Value	Unit	Source
log10ws	1.31		Crippen Method
logp	3.651		Crippen Method
rinpol	1951.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R273462&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

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<https://www.chemeo.com/cid/10-805-6/oximated-4-hydroxyphenylpyruvic-acid-diTMS.pdf>

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