

Benzenepropanoic acid, 4-[(trimethylsilyl)oxy]-«alpha»-[[trimethylsilyl]oxy] ester

Other names:

4-Hydroxyphenylpyruvic acid, oxime, tri-TMS

Phenylpyruvic acid, 4-hydroxy, oxime, tris-TMS

Pyruvic acid, 4-hydroxyphenyl, oxime, tris-TMS

Pyruvic acid, 4-hydroxyphenyl, oxime, TMS

Inchi: InChI=1S/C18H33NO4Si3/c1-24(2,3)21-16-12-10-15(11-13-16)14-17(19-23-26(7,8)9)18(

InchiKey: WKAIGQLEULMTIA-UHFFFAOYSA-N

Formula: C18H33NO4Si3

SMILES: C[Si](C)(C)ON=C(Cc1ccc(O[Si](C)(C)C)cc1)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 411.72

CAS: 55530-68-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.58		Crippen Method
logp	5.028		Crippen Method
rinpol	1954.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1938.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530682&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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