

Benzeneacetic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

Acetic acid, [m-(trimethylsiloxy)phenyl]-, trimethylsilyl ester

m-Hydroxyphenylacetic acid (tms)

Trimethylsilyl (3-[(trimethylsilyl)oxy]phenyl)acetate

3-Hydroxyphenylacetic acid, O-trimethylsilyl-, trimethylsilyl ester

3-Hydroxyphenylacetic acid, diTMS

(3-Hydroxyphenyl)acetic acid, (2TMS)-

Benzeneacetic acid, 3-hydroxy, bis-TMS

Benzeneacetic acid, 3-hydroxy, diTMS

3-Hydroxyphenylacetic acid, TMS

Benzeneacetic acid, 3-hydroxy, TMS

3-Hydroxyphenylacetic acid, 2tms derivative

Inchi:

InChI=1S/C14H24O3Si2/c1-18(2,3)16-13-9-7-8-12(10-13)11-14(15)17-19(4,5)6/h7-10H,1

InchiKey:

DIZHLFUWBKEJBT-UHFFFAOYSA-N

Formula:

C14H24O3Si2

SMILES:

C[Si](C)(C)OC(=O)Cc1cccc(O[Si](C)(C)C)c1

Mol. weight [g/mol]:

296.51

CAS:

27750-55-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.55		Crippen Method
logp	3.821		Crippen Method
rinpol	1598.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1619.00		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=C27750556&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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