

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

Other names:

o-Hydroxyphenylacetic acid (bis-TMS)
Trimethylsilyl (2-[(trimethylsilyl)oxy]phenyl)acetate
2-Hydroxyphenylacetic acid, trimethylsilyl ether, trimethylsilyl ester
2-Hydroxyphenylacetic acid diTMS
2-Hydroxyphenylacetic acid, (2TMS)
Benzeneacetic acid, 2-hydroxy, bis-TMS
2-Hydroxyphenylacetic acid, TMS
Benzeneacetic acid, 2-hydroxy, TMS
2-Hydroxybenzeneacetic acid, 2tms derivative

Inchi:

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

InchiKey:

MERYBIQYGCEFJY-UHFFFAOYSA-N

Formula:

C14H24O3Si2

SMILES:

C[Si](C)(C)OC(=O)Cc1ccccc1O[Si](C)(C)C

Mol. weight [g/mol]:

296.51

CAS:

27750-52-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.55		Crippen Method
logp	3.821		Crippen Method
rinpol	1560.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1563.40		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750523&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/42-650-3/Acetic-acid-o-trimethylsiloxy-phenyl-trimethylsilyl-ester.pdf>

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