Benzeneacetic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Acetic acid, [p-(trimethylsiloxy)phenyl]-, trimethylsilyl ester
p-Hydroxyphenylacetic acid (2TMS)
4-Hydroxyphenylacetic acid, O-trimethylsilyl-, trimethylsilyl ester
Trimethylsilyl (4-[(trimethylsilyl)oxy]phenyl)acetate
4-Hydroxyphenylacetic acid, diTMS
4-Hydroxyphenylacetic acid, bis-TMS
Benzeneacetic acid, 4-hydroxy, bis-TMS
4-Hydroxyphenylacetic acid, TMS
p-Hydroxyphenylacetic acid (tms)
4-Hydroxybenzeneacetic acid, 2tms derivative

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

InchiKey: FINLRQGHNQCJHK-UHFFFAOYSA-N

Formula: C14H24O3Si2

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

Mol. weight [g/mol]: 296.51

CAS: 27750-57-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.55		Crippen Method
logp	3.821		Crippen Method
rinpol	1629.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1633.40		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1650.00		NIST Webbook

rinpol	1648.00	NIST Webbook
rinpol	1653.00	NIST Webbook
rinpol	1648.00	NIST Webbook
rinpol	1644.00	NIST Webbook
rinpol	1649.00	NIST Webbook
rinpol	1629.00	NIST Webbook
rinpol	1650.00	NIST Webbook
rinpol	1633.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750578&Units=SI

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/61-761-9/Benzeneacetic-acid-4-trimethylsilyl-oxy-trimethylsilyl-ester.pdf
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