

Benzeneacetic acid, 2,5-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:
ester

Homogentisic acid (3TMS)

Homogentisic acid, tris(trimethylsilyl)

Benzeneacetic acid, 2,5-dihydroxy, triTMS

Homogentisic acid, bis(trimethylsilyl) ether, trimethylsilyl ester

Homogentisic acid, tri-TMS

Homogentisic acid, triTMS

Phenylacetic acid, 2,5-dihydroxy, bis(trimethylsilyl) ether, trimethylsilyl ester

Homogentisic acid, TMS

Phenylacetic acid, 2,5-dihydroxy, TMS

Benzeneacetic acid, 2,5-dihydroxy, TMS

Homogentisic acid, 3tms derivative

Inchi: InChI=1S/C17H32O4Si3/c1-22(2,3)19-15-10-11-16(20-23(4,5)6)14(12-15)13-17(18)21-22

InchiKey: NLTJSNRUCPSKFR-UHFFFAOYSA-N

Formula: C17H32O4Si3

SMILES: C[Si](C)(C)OC(=O)Cc1cc(O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 384.69

CAS: 55334-62-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.54		Crippen Method
logp	5.035		Crippen Method
rinpol	1863.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1859.00		NIST Webbook

rinpol	1841.00	NIST Webbook
rinpol	1822.70	NIST Webbook
rinpol	1834.00	NIST Webbook
rinpol	1859.00	NIST Webbook
rinpol	1853.00	NIST Webbook
rinpol	1872.00	NIST Webbook
rinpol	1822.70	NIST Webbook
rinpol	1861.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334628&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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