

Benzoic acid, 4-methoxy-, trimethylsilyl ester

Other names:	p-Anisic acid, TMS Trimethylsilyl 4-methoxybenzoate P-anisic acid, tms derivative
Inchi:	InChI=1S/C11H16O3Si/c1-13-10-7-5-9(6-8-10)11(12)14-15(2,3)4/h5-8H,1-4H3
InchiKey:	AYGQUFGXOJWAHD-UHFFFAOYSA-N
Formula:	C11H16O3Si
SMILES:	COc1ccc(C(=O)O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	224.33
CAS:	2078-14-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	2.687		Crippen Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1531.00		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=C2078140&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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