

Trimethylsilyl 2-nitrobenzoate

Other names:	2-Nitrobenzoic acid, trimethylsilyl ester 2-Nitrobenzoic acid TMS Trimethylsilyl 2-nitrobenzoate
Inchi:	InChI=1S/C10H13NO4Si/c1-16(2,3)15-10(12)8-6-4-5-7-9(8)11(13)14/h4-7H,1-3H3
InchiKey:	JVUWOCWLIHYMRJ-UHFFFAOYSA-N
Formula:	C10H13NO4Si
SMILES:	C[Si](C)(C)OC(=O)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	239.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	2.587		Crippen Method
rinpola	1566.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/10-491-5/Trimethylsilyl-2-nitrobenzoate.pdf>

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