

3,5-Dinitrobenzyl alcohol, bromomethyl dimethylsilyl ether

Inchi: InChI=1S/C10H13BrN2O5Si/c1-19(2,7-11)18-6-8-3-9(12(14)15)5-10(4-8)13(16)17/h3-5H
InchiKey: BADFRESYTLFJOF-UHFFFAOYSA-N
Formula: C10H13BrN2O5Si
SMILES: C[Si](C)(CBr)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 349.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	3.159		Crippen Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376141&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/26-199-3/3-5-Dinitrobenzyl-alcohol-bromomethyl dimethylsilyl-ether.pdf>

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