

D-(+)-Glucuronic acid «gamma»-lactone, tris(trimethylsilyl) ether, benzyloxime (isomer 1)

InChI: InChI=1S/C22H39NO6Si3/c1-30(2,3)27-18(15-23-25-16-17-13-11-10-12-14-17)19-20(28)
InChIKey: DFUOZFIYEXZVHM-UHFFFAOYSA-N
Formula: C22H39NO6Si3
SMILES: C[Si](C)(C)OC(C=NOCc1ccccc1)C1OC(=O)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 497.80

Physical Properties

Property code	Value	Unit	Source
logp	4.775		Crippen Method
rinpol	2480.80		NIST Webbook
rinpol	2480.80		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U380345&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/49-421-0/D-Glucuronic-acid-gamma-lactone-tris-trimethylsilyl-ether-benzyloxime-isomer-1>

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