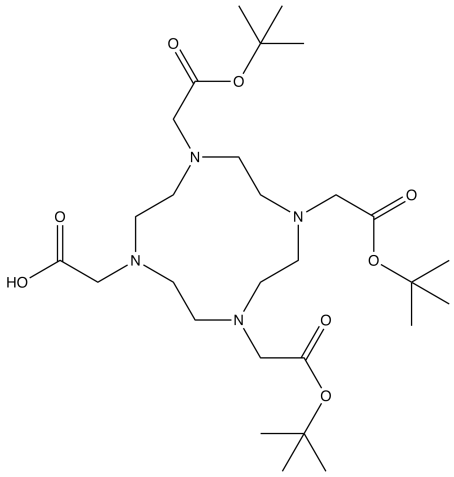
SUITE 201, 17 Ramsey Road, Shirley, NY 11967, USA
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Product Information

DOTA/*t*-Butyl ester PEG reagent, DOTA(OtBu)$_3$, Purity 95%



Cat. No.: X24-03-YW0615

Size: 50 mg; 100 mg; 250 mg

MDL: MFCD02259697

CAS Number: 137076-54-1

PubChem CID: 11606627

Synonym: 137076-54-1; Tri-*tert*-butyl 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetate; 2-(4,7,10-Tris(2-(*tert*-butoxy)-2-oxoethyl)-1,4,7,10-tetraazacyclododecan-1-yl)acetic acid; DOTA-tri(t-butyl ester); MFCD02259697

This product is for research use only and is not intended for diagnostic use.

Product Information

Description	DOTA(OtBu)$_3$ is a DOTA derivative featuring three t-butyl ester-protected carboxyl groups, enhancing stability during synthesis. The DOTA core acts as an efficient chelator for di- and trivalent metal ions, while the t-butyl esters can be selectively removed under acidic conditions.
Molecular Weight	572.7
Molecular Formula	$C_{28}H_{52}N_4O_8$
Functional Group 1	DOTA
Functional Group 2	*t*-Butyl ester
Reactive Group 1	Acid
Reactive Group 2	Chelation
IUPAC Name	2-[4,7,10-Tris[2-[(2-methylpropan-2-yl)oxy]-2-oxoethyl]-1,4,7,10-tetrazacyclododec-1-yl]acetic acid
InChI	InChI=1S/C28H52N4O8/c1-26(2,3)38-23(35)19-30-12-10-29(18-22(33)34)11-13-31(20-24(36)39-27(4,5)6)15-17-32(16-14-30)21-25(37)40-28(7,8)9/h10-21H2,1-9H3,(H,33,34)
InChI Key	RVUXZXMKYMSWOM-UHFFFAOYSA-N
Canonical SMILES	CC(C)(C)OC(=O)CN1CCN(CCN(CCN(CC1)CC(=O)OC(C)(C)C)CC(=O)OC(C)(C)C)CC(=O)OC(C)(C)C)CC(=O)O
Form	Solid
Purity	95%
Identity	Confirmed by NMR.
Applications	DOTA(OtBu)$_3$ is ideal for radiolabeling, imaging diagnostics, and metal ion chelation, allowing

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	controlled deprotection for site-specific conjugation in targeted drug delivery and biomedical research.
Storage	Store at -20°C.

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