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Typical Product Specifications & Properties

Free Isocyanates Of Isophorone Diisocynate

CAS Number: : 67873-91-0

Specifications	Limits
Molecular weight	630.82
EINECS	267-445-2
SMILES	<chem>O=C1N(c(=O)n(c(=O)n1C[C@@]1(C[C@@H](N=C=O)CC(C)(C)C1)C)C[C@@]1(C[C@@H](N=C=O)CC(C)(C)C1)C)C[C@@]1(C[C@@H](N=C=O)CC(C)(C)C1)C</chem>
InChI	BPRIYMTXVBEDNJ-UHFFFAOYSA-N
InChIKey	1S/C36H54N6O6/c1-31(2)10-25(37-22-43)13-34(7,16-31)19-40-28(46)41(20-35(8)14-26(38-23-44)11-32(3,4)17-35)30(48)42(29(40)47)21-36(9)15-27(39-24-45)12-33(5,6)18-36/h25-27H,10-21H2,1-9H3



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