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Typical Product Specifications & Properties

N-octadecyl-1,3,5-triazine-2,4,6-triamine

CAS Number: : 21840-04-0

Specifications	Limits
Chemical Structure	
Canonicalized Compound	1
Compound Complexity	305
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	3
Rotatable Bond Count	18
Allowed IUPAC Name	N2-octadecyl-1,3,5-triazine-2,4,6-triamine
CAS-like Style IUPAC Name	N2-octadecyl-1,3,5-triazine-2,4,6-triamine
Markup IUPAC Name	2- $\langle \text{I} \rangle \text{N} \langle \text{I} \rangle$ -octadecyl-1,3,5-triazine-2,4,6-triamine
Preferred IUPAC Name	2-N-octadecyl-1,3,5-triazine-2,4,6-triamine
Systematic IUPAC Name	N2-octadecyl-1,3,5-triazine-2,4,6-triamine
Traditional IUPAC Name	(4,6-diamino-s-triazin-2-yl)-stearyl-amine



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Specifications	Limits
Standard InChI	InChI=1S/C21H42N6/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-24-21-26-19(22)25-20(23)27-21/h2-18H2,1H3,(H5,22,23,24,25,26,27)
Standard InChIKey	YVQGTGVCLMMSTL-UHFFFAOYSA-N
XLogP3-AA Log P	8.4
Exact Mass	378.34709537
Molecular Weight	378.6
Canonical SMILES	CCCCCCCCCCCCCCCCCNC1=NC(=NC(=N1)N)N
Isomeric SMILES	CCCCCCCCCCCCCCCCCNC1=NC(=NC(=N1)N)N
Polar Surface Area Topological	103
Monoisotopic Weight	378.34709537



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