

2,4,6-TRI(1-AZIRIDINYL)-1,3,5-TRIAZINE

Other names:	1,3,5-Triazine, 2,4,6-tris(1-aziridinyl)- s-Triazine, 2,4,6-tris(1-aziridinyl)- Aziridine, 1,1',1''-s-triazine-2,4,6-triyltris- DRP 859025 ENT 25,296 M 9500 Melamine, triethylene- NSC-9706 Persistol Persistol Ho 1/193 Persistol Hoe 1/193 R 246 SK 1133 Tem-Simes Tretamin Tretamine Triamelin Triaziridinyl triazine Triethanomelamine Tris(ethyleneimino)triazine Trisaziridinyltriazine TAT TEM TEM (cytostatic) TET 1,1',1''-s-Triazine-2,4,6-triyltrisaziridine 2,4,6-Tri(ethyleneimino)-s-triazine 2,4,6-Tri(ethyleneimino)-1,3,5-triazine 2,4,6-Tri(ethylenimino)-s-triazine 2,4,6-Tri(ethylenimino)-1,3,5-triazine 2,4,6-Tris(ethyleneimino)-s-triazine 2,4,6-Tris(ethylenimino)-s-triazine 2,4,6-Tris(1-aziridinyl)-s-triazine 2,4,6-Tris(1-aziridinyl)-1,3,5-triazine Triaethylenmelamin 2,4,6-Tris(1'-aziridinyl)-1,3,5-triazine Trisethyleneimino-1,3,5-triazine
Inchi:	InChI=1S/C9H12N6/c1-2-13(1)7-10-8(14-3-4-14)12-9(11-7)15-5-6-15/h1-6H2
InchiKey:	IUCJMVBFZDHPDX-UHFFFAOYSA-N
Formula:	C9H12N6

SMILES: C1CN1c1nc(N2CC2)nc(N2CC2)n1
Mol. weight [g/mol]: 204.24

Physical Properties

Property code	Value	Unit	Source
logp	-0.668		Crippen Method
mcvol	141.210	ml/mol	McGowan Method

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=C51183&Units=SI>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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