(3,5-BIS-CYANOMETHYL-[1,3,5]TRIAZINAN-1-YL)-

Other names: (3,5-Bis-cyanomethyl-[1,3,5]triazinan-1-yl)-acetonitrile
1,3,5-Triazine-1,3,5(2H,4H,6H)-triacetonitrile
1,3,5-Tris(cyanomethyl)hexahydro-s-triazine
Glycinonitrile, N-methylene-,cyclictrimer
s-Triazine, hexahydro-1,3,5-tris(cyanomethyl)-
s-Triazine-1,3,5(2H,4H,6H)triacetonitrile

Inchi: InChI=1S/C9H12N6/c10-1-4-13-7-14(5-2-11)9-15(8-13)6-3-12/h4-9H2

InchiKey: CTTRIWVSECLRDA-UHFFFAOYSA-N

Formula: C9H12N6

SMILES: N#CCN1CN(CC#N)CN(CC#N)C1

Mol. weight [g/mol]: 204.24

Physical Properties

Property code	Value	Unit	Source
hf	452.46	kJ/mol	Cheméo Relay (1.0)
logp	-0.651		Crippen Method
mcvol	160.890	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4560876&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume