1,3,5-Tris(cyanomethyl)-S-hexahydrotriazine

Other names:	s-Triazine-1,3,5(2H,4H,6H)triacetonitrile
	s-Triazine, hexahydro-1,3,5-tris(cyanomethyl)-
	1,3,5-Tris(cyanomethyl)hexahydro-s-triazine
	1,3,5-Triazine-1,3,5(2H,4H,6H)-triacetonitrile
	(3,5-Bis-cyanomethyl-[1,3,5]triazinan-1-yl)-acetonitrile
	Glycinonitrile, N-methylene-,cyclictrimer
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]:	204.23
CAS:	4560-87-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.28		Crippen Method
logp	-0.651		Crippen Method
mcvol	160.890	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4560876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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