

S-triazine, 2,4,6-triazido-

Inchi:	InChI=1S/C3N12/c4-13-10-1-7-2(11-14-5)9-3(8-1)12-15-6
InchiKey:	JKYMSKUDZIJFKI-UHFFFAOYSA-N
Formula:	C3N12
SMILES:	[N-]=[N+]=Nc1nc(N=[N+]=[N-])nc(N=[N+]=[N-])n1
Mol. weight [g/mol]:	204.11
CAS:	5637-83-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-17.74		Crippen Method
logp	2.697		Crippen Method
mcvol	123.330	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5637832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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