

S-triazine], 2,2'-cyclobut-1,2-ylene-bis[4,6-diamino-

Inchi:	InChI=1S/C10H14N10/c11-7-15-5(16-8(12)19-7)3-1-2-4(3)6-17-9(13)20-10(14)18-6/h3-4
InchiKey:	WJMJAVJXAOBTAX-UHFFFAOYSA-N
Formula:	C10H14N10
SMILES:	Nc1nc(N)nc(C2CCC2c2nc(N)nc(N)n2)n1
Mol. weight [g/mol]:	274.29
CAS:	19438-85-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	-0.953		Crippen Method
mcvol	193.180	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19438858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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