1,2,4,5-Tetrazine

Other names:	s-Tetrazine
	sym-Tetrazine
Inchi:	InChI=1S/C2H2N4/c1-3-5-2-6-4-1/h1-2H
InchiKey:	HTJMXYRLEDBSLT-UHFFFAOYSA-N
Formula:	C2H2N4
SMILES:	c1nncnn1
Mol. weight [g/mol]:	82.06
CAS:	290-96-0

Physical Properties

Property code	Value	Unit	Source
ie	9.14	eV	NIST Webbook
ie	9.24	eV	NIST Webbook
log10ws	-0.53		Crippen Method
logp	-0.733		Crippen Method
mcvol	55.200	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=C290960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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https://www.chemeo.com/cid/30-708-2/1-2-4-5-Tetrazine.pdf

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