

1,2,4-Benzotriazin-3(4h)-one, 4(hydroxymethyl)-

Inchi:	InChI=1S/C8H7N3O2/c12-5-11-7-4-2-1-3-6(7)9-10-8(11)13/h1-4,12H,5H2
InchiKey:	QJCSBGIUQSSKHX-UHFFFAOYSA-N
Formula:	C8H7N3O2
SMILES:	O=c1nnc2ccccc2n1CO
Mol. weight [g/mol]:	177.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	-0.259		Crippen Method
mcvol	122.040	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=B6008076&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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