

Pyrido[2,3-d]pyridazine

Other names:	1,6,7-Triazanaphthalene
Inchi:	InChI=1S/C7H5N3/c1-2-6-4-9-10-5-7(6)8-3-1/h1-5H
InchiKey:	GIVUQTUKKWDKHE-UHFFFAOYSA-N
Formula:	C7H5N3
SMILES:	c1cnc2cncc2c1
Mol. weight [g/mol]:	131.13
CAS:	253-73-6

Physical Properties

Property code	Value	Unit	Source
ea	1.00 ± 0.10	eV	NIST Webbook
log10ws	-2.57		Crippen Method
logp	1.025		Crippen Method
mcvol	96.210	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C253736&Units=SI

Legend

ea:	Electron affinity
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/51-588-3/Pyrido-2-3-d-pyridazine.pdf>

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