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: c1cnc2cnncc2c1
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/ci990307l
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