

2,3-Cycloheptenopyridine

Other names:	5H-Cyclohepta[b]pyridine, 6,7,8,9-tetrahydro-6,7,8,9-tetrahydro-5H-cyclohepta(b)pyridine
Inchi:	InChI=1S/C10H13N/c1-2-5-9-6-4-8-11-10(9)7-3-1/h4,6,8H,1-3,5,7H2
InchiKey:	CULUYAUTCSKQNM-UHFFFAOYSA-N
Formula:	C10H13N
SMILES:	c1cnc2c(c1)CCCCC2
Mol. weight [g/mol]:	147.22
CAS:	7197-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.350		Crippen Method
mcvol	127.120	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7197968&Units=SI

Legend

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

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