1H-Pyrazolo[4,3-d]pyrimidin-7-amine

Other names:	1H-Pyrazolo[4,3-d]pyrimidine, 7-amino- 7-Aminopyrazolo[4,3-d]-pyrimidine
Inchi:	InChI=1S/C5H5N5/c6-5-4-3(1-9-10-4)7-2-8-5/h1-2H,(H,9,10)(H2,6,7,8)
InchiKey:	MPDXYVOXVJOKIN-UHFFFAOYSA-N
Formula:	C5H5N5
SMILES:	Nc1ncnc2c[nH]nc12
Mol. weight [g/mol]:	135.13
CAS:	13877-56-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	-0.547		Crippen Method
mcvol	92.290	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=C13877560&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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