

Imidazole-5-carboxylic amide, 4-acetamino-

Other names:	Imidazole-5-carboxamide, 4-acetamido-
Inchi:	InChI=1S/C6H8N4O2/c1-3(11)10-6-4(5(7)12)8-2-9-6/h2H,1H3,(H2,7,12)(H,8,9)(H,10,11)
InchiKey:	JNCFMTGDCURKGM-UHFFFAOYSA-N
Formula:	C6H8N4O2
SMILES:	CC(=O)Nc1nc[nH]c1C(N)=O
Mol. weight [g/mol]:	168.15
CAS:	91026-74-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
logp	-1.015		Crippen Method
mcvol	119.000	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91026743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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