

Acetamide, n-[4(5)-imidazolyl]-

Inchi:	InChI=1S/C5H7N3O/c1-4(9)8-5-2-6-3-7-5/h2-3H,1H3,(H,6,7)(H,8,9)
InchiKey:	GKFMAGUWGRNGIW-UHFFFAOYSA-N
Formula:	C5H7N3O
SMILES:	CC(=O)Nc1c[nH]cn1
Mol. weight [g/mol]:	125.13
CAS:	51741-72-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.66		Crippen Method
logp	-0.114		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51741721&Units=SI
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

Legend

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/45-164-0/Acetamide-n-4-5-imidazolyl.pdf>

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