

Formamide, n-2-pyrimidinyl-

Inchi:	InChI=1S/C5H5N3O/c9-4-8-5-6-2-1-3-7-5/h1-4H,(H,6,7,8,9)
InchiKey:	ANCSTOBSCOWSPF-UHFFFAOYSA-N
Formula:	C5H5N3O
SMILES:	O=CNC1NCCCN1
Mol. weight [g/mol]:	123.11
CAS:	31354-57-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.79		Crippen Method
logp	0.045		Crippen Method
mcvol	89.060	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=C31354571&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/44-828-4/Formamide-n-2-pyrimidinyl.pdf>

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