

Pyrimidine, 5-amino-4- (ethylamino)-

Inchi:	InChI=1S/C6H10N4/c1-2-9-6-5(7)3-8-4-10-6/h3-4H,2,7H2,1H3,(H,8,9,10)
InchiKey:	RLRUJMDXPFHVDE-UHFFFAOYSA-N
Formula:	C6H10N4
SMILES:	CCN=c1[nH]cncc1N
Mol. weight [g/mol]:	138.17
CAS:	101080-16-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.17		Crippen Method
logp	-0.569		Crippen Method
mcvol	111.560	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=C101080164&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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