

Pyrimidine, 2,5-diamino-

Inchi:	InChI=1S/C4H6N4/c5-3-1-7-4(6)8-2-3/h1-2H,5H2,(H2,6,7,8)
InchiKey:	DNACGYGXUFTEHO-UHFFFAOYSA-N
Formula:	C4H6N4
SMILES:	Nc1cnc(N)nc1
Mol. weight [g/mol]:	110.12
CAS:	22715-27-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.27		Crippen Method
logp	-0.359		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22715271&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/11-288-0/Pyrimidine-2-5-diamino.pdf>

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