4,5-Pyrimidinediamine

Other names:	Pyrimidine, 4,5-diamino- 4,5-Diaminopyrimidine Pyrimidine-4,5-diamine
Inchi:	InChI=1S/C4H6N4/c5-3-1-7-2-8-4(3)6/h1-2H,5H2,(H2,6,7,8)
InchiKey:	PPAULTVPKLVLII-UHFFFAOYSA-N
Formula:	C4H6N4
SMILES:	N=c1[nH]cncc1N
Mol. weight [g/mol]:	110.12
CAS:	13754-19-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	-1.011		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	502.20	K	4.30	NIST Webbook

Sources

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=C13754193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure