2-amino-4,6-dichloropyrimidine

Inchi: InChI=1S/C4H3Cl2N3/c5-2-1-3(6)9-4(7)8-2/h1H,(H2,7,8,9)
InchiKey: JPZOAVGMSDSWSW-UHFFFAOYSA-N
Formula: C4H3Cl2N3
SMILES: Nc1nc(Cl)cc(Cl)n1
Mol. weight [g/mol]: 164.00

Physical Properties

Property code	Value	Unit	Source
hfus	19.50	kJ/mol	Solubility Measurement and Modeling of 2-Amino-4,6-dichoropyrimidine in Ten Pure Solvents and (Ethyl Acetate + Ethanol) Solvent Mixtures
log10ws	-2.01		Crippen Method
logp	1.366		Crippen Method
mcvol	97.880	ml/mol	McGowan Method
tt	496.42	K	Solubility Measurement and Modeling of 2-Amino-4,6-dichoropyrimidine in Ten Pure Solvents and (Ethyl Acetate + Ethanol) Solvent Mixtures

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Solubility Measurement and Modeling of 2-Amino-4,6-dichoropyrimidine in Ten Pure Solvents and (Ethyl Acetate + Ethanol) Solvent Mixtures: https://www.doi.org/10.1021/acs.jced.8b00292
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tt:	Triple Point Temperature