

5-Amino-4,6-dichloropyrimidine

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| Other names: | 5-Pyrimidinamine, 4,6-dichloro-Pyrimidine, 5-amino-4,6-dichloro-4,6-Dichloro-5-aminopyrimidine, 4,6-Dichloro-5-pyrimidinamine, 4,6-Dichloropyrimidin-5-ylamine |
| Inchi: | InChI=1S/C4H3Cl2N3/c5-3-2(7)4(6)9-1-8-3/h1H,7H2 |
| InchiKey: | NIGDWBHWHVHOAD-UHFFFAOYSA-N |
| Formula: | C4H3Cl2N3 |
| SMILES: | Nc1c(Cl)ncnc1Cl |
| Mol. weight [g/mol]: | 163.99 |
| CAS: | 5413-85-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -2.01 | | Crippen Method |
| logp | 1.366 | | Crippen Method |
| mcvol | 97.880 | ml/mol | McGowan Method |

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=C5413854&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 |

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