

Pyrimidine, 5-amino-6-chloro-4-(methylamino)-

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C5H7ClN4/c1-8-5-3(7)4(6)9-2-10-5/h2H,7H2,1H3,(H,8,9,10) |
| InchiKey: | RIYBSFHJIOZYLD-UHFFFAOYSA-N |
| Formula: | C5H7ClN4 |
| SMILES: | CNc1ncnc(Cl)c1N |
| Mol. weight [g/mol]: | 158.59 |
| CAS: | 52602-68-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.33 | | Crippen Method |
| logp | 0.754 | | Crippen Method |
| mcvol | 109.710 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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=C52602683&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

Latest version available from:

<https://www.chemeo.com/cid/37-718-4/Pyrimidine-5-amino-6-chloro-4-methylamino.pdf>

Generated by Cheméo on 2024-04-27 03:45:52.277618691 +0000 UTC m=+16478801.198196003.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.