

Pyrimidine, 5-amino-6-chloro-2-ethyl-4-ethylamino-

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|-----------------------------|--|
| Inchi: | InChI=1S/C8H13ClN4/c1-3-5-12-7(9)6(10)8(13-5)11-4-2/h3-4,10H2,1-2H3,(H,11,12,13) |
| InchiKey: | CTGPZVJZVOTQRL-UHFFFAOYSA-N |
| Formula: | C8H13ClN4 |
| SMILES: | CCNc1nc(CC)nc(Cl)c1N |
| Mol. weight [g/mol]: | 200.67 |
| CAS: | 6237-98-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.55 | | Crippen Method |
| logp | 1.706 | | Crippen Method |
| mcvol | 151.980 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6237985&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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