

Purine, 6-dimethylamino-2-methylamino-

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|-----------------------------|---|
| Inchi: | InChI=1S/C8H12N6/c1-9-8-12-6-5(10-4-11-6)7(13-8)14(2)3/h4H,1-3H3,(H2,9,10,11,12,13) |
| InchiKey: | LXLSAAOQPMAASG-UHFFFAOYSA-N |
| Formula: | C8H12N6 |
| SMILES: | CNc1nc(N(C)C)c2[nH]cnc2n1 |
| Mol. weight [g/mol]: | 192.22 |
| CAS: | 101251-43-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.71 | | Crippen Method |
| logp | -0.021 | | Crippen Method |
| mcvol | 144.540 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C101251438&Units=SI |

Legend

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

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<https://www.chemeo.com/cid/11-191-7/Purine-6-dimethylamino-2-methylamino.pdf>

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