

# 2,4(1H,3H)-Pyrimidinedione, 5-[bis(2-chloroethyl)amino]-

Other names: 2,4(1H,3H)-Pyrimidinedione, 5-[bis(2-chloroethyl)amino]-  
Uracil, 5-[bis(2-chloroethyl)amino]-  
Aminouracil mustard  
Chlorethaminacil  
Demethyldopan  
Desmethyldopan  
ENT 50439  
Nordopan  
NSC-34462  
U-8344  
Uracillost  
Uracilmostaza  
Uramustin  
Uramustine  
2,6-Dihydroxy-5-[bis(2-chloroethyl)amino]pyrimidine  
5-[Bis(2-chloroethyl)amino]uracil  
5-[Di(«beta»-chloroethyl)amino]uracil  
CB-4835  
NCI-C04820  
SK-19849  
Uracil nitrogen mustard  
5-(Bis(2-chlorethyl)amino)-2,4(1H,3H)pyrimidinedione  
5-(Di(2-chloroethyl)amino)uracil  
5-(Bis(2-chloroethyl)amino)-2,4(1H,3H)pyrimidinedione  
5-N,N-Bis(2-chloroethyl)aminouracil  
Rcra waste number U237

**Inchi:** InChI=1S/C8H11Cl2N3O2/c9-1-3-13(4-2-10)6-5-11-8(15)12-7(6)14/h5H,1-4H2,(H2,11,12)  
**InchiKey:** IDPUKCWIGUEADI-UHFFFAOYSA-N  
**Formula:** C8H11Cl2N3O2  
**SMILES:** O=c1[nH]cc(N(CCCl)CCCl)c(=O)[nH]1  
**Mol. weight [g/mol]:** 252.10

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | -0.617  |        | Crippen Method |
| mcvol         | 165.980 | ml/mol | McGowan Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C66751&Units=SI>

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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