

1H-Pyrazolo[4,3-d]pyrimidine, 7-amino-3-«beta»-D-ribofuranosyl-

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|-----------------------------|---|
| Other names: | D-Ribitol, 1-C-(7-amino-1H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- Formycin Formycin A 7-Amino-3-«beta»-D-ribofuranosyl-1H-pyrazolo(4,3-d)pyrimidine |
| Inchi: | InChI=1S/C10H13N5O4/c11-10-6-4(12-2-13-10)5(14-15-6)9-8(18)7(17)3(1-16)19-9/h2-3 |
| InchiKey: | KBHMEHLJSZMEMI-UHFFFAOYSA-N |
| Formula: | C10H13N5O4 |
| SMILES: | <chem>Nc1ncnc2c(C3OC(CO)C(O)C3O)n[nH]c12</chem> |
| Mol. weight [g/mol]: | 267.24 |
| CAS: | 6742-12-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.05 | | Crippen Method |
| logp | -2.393 | | Crippen Method |
| mcvol | 175.360 | 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=C6742127&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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