

7,9,10-Tri-hydroxy-1,5-iso-phenazine

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H8N2O3/c15-6-4-8-10(9(16)5-6)12(17)11-7(14-8)2-1-3-13-11/h1-5,15-16H |
| InchiKey: | QZWTWYKVVOWIBI-UHFFFAOYSA-N |
| Formula: | C12H8N2O3 |
| SMILES: | Oc1cc(O)c2c(O)c3ncccc3nc2c1 |
| Mol. weight [g/mol]: | 228.20 |
| CAS: | 116495-78-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.26 | | Crippen Method |
| logp | 1.900 | | Crippen Method |
| mcvol | 154.830 | 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=C116495784&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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