

1-Isopropenyl-2-benzimidazolinone

| | |
|-----------------------------|--|
| Other names: | 1,3-dihydro-1-(1-methylvinyl)-2H-benzimidazol-2-one |
| Inchi: | InChI=1S/C10H10N2O/c1-7(2)12-9-6-4-3-5-8(9)11-10(12)13/h3-6H,1H2,2H3,(H,11,13) |
| InchiKey: | XFASJWL BXHWUMW-UHFFFAOYSA-N |
| Formula: | C10H10N2O |
| SMILES: | C=C(C)n1c(O)nc2ccccc21 |
| Mol. weight [g/mol]: | 174.20 |
| CAS: | 52099-72-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.29 | | Crippen Method |
| logp | 2.232 | | Crippen Method |
| mcvol | 134.370 | 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=C52099726&Units=SI |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/94-449-0/1-Isopropenyl-2-benzimidazolinone.pdf>

Generated by Cheméo on 2024-04-27 04:24:18.777367797 +0000 UTC m=+16481107.697945117.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.