

RTI 23

Inchi: InChI=1S/C16H17N3O2/c1-4-19-13-9-11(21-3)8-10(2)14(13)18-16(20)12-6-5-7-17-15(12)
InchiKey: PVVKNINYCJVIFZ-UHFFFAOYSA-N
Formula: C16H17N3O2
SMILES: CCN1c2cc(OC)cc(C)c2NC(=O)c2cccnc21
Mol. weight [g/mol]: 283.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|-----------------------------|
| log10ws | -5.15 | | Estimated Solubility Method |
| logp | 3.122 | | Crippen Method |
| mcvol | 215.300 | ml/mol | McGowan Method |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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.cheméo.com/cid/102-423-8/RTI-23.pdf>

Generated by Cheméo on 2024-04-27 21:31:08.675780174 +0000 UTC m=+16542717.596357493.

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