

irbesartan

Inchi: InChI=1S/C25H28N6O/c1-2-3-10-22-26-25(15-6-7-16-25)24(32)31(22)17-18-11-13-19(14)
InchiKey: YOSHYTLCDANDAN-UHFFFAOYSA-N
Formula: C25H28N6O
SMILES: CCCCC1=NC2(CCCC2)C(=O)N1Cc1ccc(-c2ccccc2-c2nn[nH]n2)cc1
Mol. weight [g/mol]: 428.54

Physical Properties

Property code	Value	Unit	Source
logp	4.296		Crippen Method
mcvol	331.560	ml/mol	McGowan Method

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Solubility of Irbesartan (Form A) in Different Solvents between 278 K and 325 K: <https://www.doi.org/10.1021/je700296x>
Solubility of Irbesartan Form B in an Aqueous Ethanol Mixture: <https://www.doi.org/10.1021/je700627z>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/110-705-6/irbesartan.pdf>

Generated by Cheméo on 2026-07-21 09:52:38.494882129 +0000 UTC m=+138654.336767538.

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