

Allopurinol

Other names: 1,5-Dihydro-4H-pyrazolo(3,4-d)pyrimidin-4-one
1H-Pyrazolo[3,4-d]Pyrimidin-4-ol
4'-Hydroxypyrazolol(3,4-d)pyrimidine
4-HPP
4-Hydroxy-1H-pyrazolo[3,4-d]pyrimidine
4-Hydroxy-3,4-pyrazolopyrimidine
4-Hydroxypyrazolo[3,4-d]pyrimidine
4-Hydroxypyrazolopyrimidine
4-Hydroxypyrazolyl(3,4-d)pyrimidine
4H-Pyrazolo(3,4-d)pyrimidin-4-one
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-
AL-100
Adenock
Ailural
Allopur
Allopurinol(l)
Allozym
Allural
Aloral
Alositol
Aluline
Anoprolin
Anzief
Apurin
Apurol
Atisuril
B. W. 56-158
BW 56-158
Bleminol
Bloxanth
Caplenal
Cellidrin
Cosuric
Dabrosin
Dabroson
Embarin
Epidropal
Foligan
Geapur
Gichtex

Gotax
HPP
Hamarin
Hexanurat
Ketanrift
Ketobun-A
Ledopur
Lopurin
Lysuron
Milurit
Miniplanor
Monarch
NSC-1390
Nektrohan
Progout
Remid
Riball
Sigapurol
Suspendol
Takanarumin
Urbol
Uricemil
Uriprim
Uripurinol
Uritas
Urobenyl
Urolit
Urosin
Urtias
Xanturat
Zyloprim
Zyloric

Inchi: InChI=1S/C5H4N4O/c10-5-3-1-8-9-4(3)6-2-7-5/h1-2H,(H2,6,7,8,9,10)
InchiKey: OFCNXP DARWKPPY-UHFFFAOYSA-N
Formula: C5H4N4O
SMILES: O=c1[nH]cnc2[nH]ncc12
Mol. weight [g/mol]: 136.11
CAS: 315-30-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.23		Aqueous Solubility Prediction Method
log10ws	-2.27		Estimated Solubility Method
logp	-1.318		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
rinpol	882.00		NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>

Solubility modelling and thermodynamic properties of allopurinol in neat solvents: <https://www.doi.org/10.1016/j.jct.2019.01.018>

Solubility modelling and solvent effect of allopurinol in neat solvents: <https://www.doi.org/10.1021/acs.jced.8b00430>

Aqueous Solubility Prediction Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307i>

NIST Webbook: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C315300&Units=SI>

Estimated Solubility Method: <http://link.springer.com/article/10.1007/BF02311772>

Solubility modelling, solvent effect and preferential solvation of allopurinol in aqueous cosolvent mixtures of ethanol, isopropanol, N,N-dimethylformamide and 1-methyl-2-pyrrolidone: <https://www.doi.org/10.1016/j.jct.2018.11.028>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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