Azathioprine

Inchi: InChI=1S/C9H7N7O2S/c1-15-4-14-7(16(17)18)9(15)19-8-5-6(11-2-10-5)12-3-13-8/h2-4H
InchiKey: LMEKQMALGUDUQG-UHFFFAOYSA-N
Formula: C9H7N7O2S
SMILES: Cn1cnc([N+](=O)[O-])c1Sc1ncnc2nc[nH]c12
Mol. weight [g/mol]: 277.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Aqueous Solubility Prediction Method
log10ws	-3.44		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.664		Crippen Method
mcvol	172.940	ml/mol	McGowan Method
tf	492.65	K	Aqueous Solubility Prediction Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point