Hypoxanthine, 1-allyl-9-benzyl-

Inchi: InChI=1S/C15H14N4O/c1-2-8-18-11-17-14-13(15(18)20)16-10-19(14)9-12-6-4-3-5-7-12/h
InchiKey: KGDYVANAUGZTCM-UHFFFAOYSA-N
Formula: C15H14N4O
SMILES: C=CCn1cnc2c(ncn2Cc2ccccc2)c1=O
Mol. weight [g/mol]: 266.30
CAS: 108160-10-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	1.827		Crippen Method
mcvol	201.020	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108160107&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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