Purine-6(3h)-one, 3-benzyl-

Inchi: InChI=1S/C12H10N4O/c17-12-10-11(14-7-13-10)16(8-15-12)6-9-4-2-1-3-5-9/h1-5,7-8H,6

InchiKey: CSUJRAOXOXPOHI-UHFFFAOYSA-N

Formula: C12H10N4O

SMILES: O=c1ncn(Cc2ccccc2)c2nc[nH]c12

Mol. weight [g/mol]: 226.23

CAS: 3649-39-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	0.686		Crippen Method
mcvol	163.050	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3649396&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume