

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

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<https://www.chemeo.com/cid/66-319-5/Purine-6-3h-one-3-benzyl.pdf>

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