

Purine, 2,6-bis(benzamido)-

Inchi:	InChI=1S/C19H14N6O2/c26-17(12-7-3-1-4-8-12)22-16-14-15(21-11-20-14)23-19(24-16)
InchiKey:	OGTOITXPCGGWSB-UHFFFAOYSA-N
Formula:	C19H14N6O2
SMILES:	O=C(Nc1nc(NC(=O)c2ccccc2)c2nc[nH]c2n1)c1ccccc1
Mol. weight [g/mol]:	358.35
CAS:	51173-57-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	2.376		Crippen Method
mcvol	255.150	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51173570&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/122-865-6/Purine-2-6-bis-benzamido.pdf>

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