

Imidazole-5-formamide, n,1-dibenzyl-4-(n-benzylformamido)-

Inchi:	InChI=1S/C26H24N4O2/c31-20-30(18-23-14-8-3-9-15-23)25-24(26(32)27-16-21-10-4-1-5
InchiKey:	NHTKENXXMKCBAY-UHFFFAOYSA-N
Formula:	C26H24N4O2
SMILES:	O=CN(Cc1ccccc1)c1ncn(Cc2ccccc2)c1C(=O)NCc1ccccc1
Mol. weight [g/mol]:	424.49
CAS:	7026-46-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.04		Crippen Method
logp	4.024		Crippen Method
mcvol	329.520	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=C7026462&Units=SI

Legend

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

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