

Imidazole-4-carboxamide, 1-benzyl-5-(n-benzylformamido)-

Inchi:	InChI=1S/C19H18N4O2/c20-18(25)17-19(23(14-24)12-16-9-5-2-6-10-16)22(13-21-17)11
InchiKey:	HNHCJLBTDCNI-UHFFFAOYSA-N
Formula:	C19H18N4O2
SMILES:	NC(=O)c1ncn(Cc2ccccc2)c1N(C=O)Cc1ccccc1
Mol. weight [g/mol]:	334.37
CAS:	7178-28-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	2.193		Crippen Method
mcvol	254.650	ml/mol	McGowan Method

Sources

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=C7178281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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