

Imidazole-4-carboxamide, 1-benzyl-5-(benzylamino)-

Inchi:	InChI=1S/C18H18N4O/c19-17(23)16-18(20-11-14-7-3-1-4-8-14)22(13-21-16)12-15-9-5-2
InchiKey:	IKOPTFPVYMQQLP-UHFFFAOYSA-N
Formula:	C18H18N4O
SMILES:	NC(=O)c1ncn(Cc2ccccc2)c1NCc1ccccc1
Mol. weight [g/mol]:	306.36
CAS:	7026-48-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	2.642		Crippen Method
mcvol	238.990	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7026484&Units=SI
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

Legend

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

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