

Imidazole-4(or 5)-carboxamide, n-benzyl-5(or 4)-(benzylamino)-

Inchi:	InChI=1S/C18H18N4O/c23-18(20-12-15-9-5-2-6-10-15)16-17(22-13-21-16)19-11-14-7-3
InchiKey:	JEWIFRZMMFFXCZ-UHFFFAOYSA-N
Formula:	C18H18N4O
SMILES:	OC(=NCc1cccc1)c1nc[nH]c1NCc1cccc1
Mol. weight [g/mol]:	306.36
CAS:	116373-95-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	3.045		Crippen Method
mvol	238.990	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=C116373956&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
mvol:	McGowan's characteristic volume

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