2-Benzylideneamino-2,1,3-benzotriazole

Inchi:	InChI=1S/C13H10N4/c1-2-6-11(7-3-1)10-14-17-15-12-8-4-5-9-13(12)16-17/h1-10H
InchiKey:	JHHYYGTUYDAKCM-UHFFFAOYSA-N
Formula:	C13H10N4
SMILES:	C(=Nn1nc2ccccc2n1)c1ccccc1
Mol. weight [g/mol]:	222.25
CAS:	21978-61-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	2.313		Crippen Method
mcvol	166.970	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21978610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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