4H-1,2,4-Triazol-4-amine, N-(phenylmethylene)-

Other names: 4-Benzylideneamino-4H-1,2,4-triazole
[1,2,4]Triazole, 4-benzylidenamino-
Inchi: InChI=1S/C9H8N4/c1-2-4-9(5-3-1)6-12-13-7-10-11-8-13/h1-8H
InchiKey: VBIZJJNFYLXNBK-UHFFFAOYSA-N
Formula: C9H8N4
SMILES: C(=Nn1cnnc1)c1ccccc1
Mol. weight [g/mol]: 172.19
CAS: 18998-48-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	1.160		Crippen Method
mcvol	130.070	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=C18998486&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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