1-Benzyl-1,2,3-triazole

Inchi: InChI=1S/C9H9N3/c1-2-4-9(5-3-1)8-12-7-6-10-11-12/h1-7H,8H2
InchiKey: VRDSRXVCRBMZOD-UHFFFAOYSA-N
Formula: C9H9N3
SMILES: c1ccc(Cn2ccnn2)cc1
Mol. weight [g/mol]: 159.19
CAS: 4368-68-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.326		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4368687&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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