1H-[1,2,3]triazole-4-carboxamide, 5-amino-1-(phenylmethyl)-

Other names: 1H-[1,2,3]Triazole-4-carboxamide, 5-amino-1-benzyl-
Inchi: InChI=1S/C10H11N5O/c11-9-8(10(12)16)13-14-15(9)6-7-4-2-1-3-5-7/h1-5H,6,11H2,(H2,
InchiKey: SPSJTSUTONSWEX-UHFFFAOYSA-N
Formula: C10H11N5O
SMILES: NC(=O)c1nnn(Cc2ccccc2)c1N
Mol. weight [g/mol]: 217.23

Physical Properties

Property code	Value	Unit	Source
logp	0.008		Crippen Method
mcvol	160.010	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4342089&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume