

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
CAS:	4342-08-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	0.008		Crippen Method
mcvol	160.010	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4342089&Units=SI

Legend

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

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