

Triazole-4-carboxylic acid, 3h-1,2,3-, 5-amino-3-phenyl-, ethyl ester

Inchi:	InChI=1S/C11H12N4O2/c1-2-17-11(16)9-10(12)13-14-15(9)8-6-4-3-5-7-8/h3-7H,2,12H2,
InchiKey:	KYWFKGSZLZLJKF-UHFFFAOYSA-N
Formula:	C11H12N4O2
SMILES:	CCOC(=O)c1c(N)nnn1-c1ccccc1
Mol. weight [g/mol]:	232.24
CAS:	116632-73-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	1.026		Crippen Method
mcvol	169.990	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116632736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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