

Triazolo[4,5-d]pyrimidine, 1h-v-, 5-amino-7-ethoxy-

Inchi:	InChI=1S/C6H8N6O/c1-2-13-5-3-4(11-12-10-3)8-6(7)9-5/h2H2,1H3,(H3,7,8,9,10,11,12)
InchiKey:	JIAFSVYUQOFABK-UHFFFAOYSA-N
Formula:	C6H8N6O
SMILES:	CCOc1nc(N)nc2nn[nH]c12
Mol. weight [g/mol]:	180.17
CAS:	91314-05-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	-0.753		Crippen Method
mcvol	122.230	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=C91314055&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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