

# Triazolo [4,5-d]pyrimidine, 3h-v-, 5,7-diamino-3-ethyl-

Inchi:	InChI=1S/C6H9N7/c1-2-13-5-3(11-12-13)4(7)9-6(8)10-5/h2H2,1H3,(H4,7,8,9,10)
InchiKey:	YTUXGRIGGVSGDJ-UHFFFAOYSA-N
Formula:	C6H9N7
SMILES:	CCn1nnc2c(N)nc(N)nc21
Mol. weight [g/mol]:	179.18
CAS:	7256-20-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.87		Crippen Method
logp	-0.594		Crippen Method
mcvol	126.340	ml/mol	McGowan Method

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7256204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7256204&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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