

Triazolo[4,5-d]pyrimidine, 3h-v-, 5-amino-7-chloro-3-ethyl-

Inchi:	InChI=1S/C6H7ClN6/c1-2-13-5-3(11-12-13)4(7)9-6(8)10-5/h2H2,1H3,(H2,8,9,10)
InchiKey:	DTOBYQFBYWOFFC-UHFFFAOYSA-N
Formula:	C6H7ClN6
SMILES:	CCn1nnc2c(Cl)nc(N)nc21
Mol. weight [g/mol]:	198.61
CAS:	5457-92-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	0.477		Crippen Method
mcvol	128.600	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=C5457921&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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