

1H-Tetrazol-5-amine, N-ethyl-

Inchi:	InChI=1S/C3H7N5/c1-2-4-3-5-7-8-6-3/h2H2,1H3,(H2,4,5,6,7,8)
InchiKey:	AYZFMCOIISJDHU-UHFFFAOYSA-N
Formula:	C3H7N5
SMILES:	CCN=c1nn[nH][nH]1
Mol. weight [g/mol]:	113.12
CAS:	118725-48-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	-1.910		Crippen Method
mcvol	83.570	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=C118725487&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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<https://www.chemeo.com/cid/81-290-0/1H-Tetrazol-5-amine-N-ethyl.pdf>

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