

1H-1,2,4-Triazol-5-amine, 1-ethyl-

Inchi:	InChI=1S/C4H8N4/c1-2-8-4(5)6-3-7-8/h3H,2H2,1H3,(H2,5,6,7)
InchiKey:	SXRAEXLYRRHOSI-UHFFFAOYSA-N
Formula:	C4H8N4
SMILES:	CCn1ncnc1N
Mol. weight [g/mol]:	112.13
CAS:	58661-94-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.90		Crippen Method
logp	-0.120		Crippen Method
mcvol	87.680	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=C58661942&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/21-082-7/1H-1-2-4-Triazol-5-amine-1-ethyl.pdf>

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