

4H-1,2,4-Triazol-3-amine, 4-ethyl-

Other names:	4H-1,2,4-Triazole, 3-amino-4-ethyl-
Inchi:	InChI=1S/C4H8N4/c1-2-8-3-6-7-4(8)5/h3H,2H2,1H3,(H2,5,7)
InchiKey:	OTXAZICPXWFRME-UHFFFAOYSA-N
Formula:	C4H8N4
SMILES:	CCn1cnnc1N
Mol. weight [g/mol]:	112.13
CAS:	42786-06-1

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	-0.120		Crippen Method
mcvol	87.680	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=C42786061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
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/69-394-9/4H-1-2-4-Triazol-3-amine-4-ethyl.pdf>

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