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/ci990307l

Legend

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