

# 7-ethyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ETBD)

**Inchi:** InChI=1S/C9H17N3/c1-2-11-7-4-8-12-6-3-5-10-9(11)12/h2-8H2,1H3  
**InchiKey:** AAPJUEKLMYSSCH-UHFFFAOYSA-N  
**Formula:** C9H17N3  
**SMILES:** CCN1CCCN2CCCN=C12  
**Mol. weight [g/mol]:** 167.25  
**CAS:** 95510-44-4

## Physical Properties

Property code	Value	Unit	Source
affp	1068.20	kJ/mol	NIST Webbook
basg	1035.80	kJ/mol	NIST Webbook
log10ws	-0.67		Crippen Method
logp	0.774		Crippen Method
mcvol	141.590	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=C95510444&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**affp:** Proton affinity  
**basg:** Gas basicity  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/60-914-0/7-ethyl-1-5-7-triazabicyclo-4-4-0-dec-5-ene-ETBD.pdf>

Generated by Cheméo on 2024-04-17 01:44:56.278552881 +0000 UTC m=+15607545.199130193.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.