

# Cyanoethynyl radical

**Inchi:** InChI=1S/C3N/c1-2-3-4  
**InchiKey:** URBHYAWCGWIELS-UHFFFAOYSA-N  
**Formula:** C3N  
**SMILES:** [C]#CC#N  
**Mol. weight [g/mol]:** 50.04  
**CAS:** 12543-75-8

## Physical Properties

Property code	Value	Unit	Source
ea	4.30 ± 0.00	eV	NIST Webbook
ea	4.43 ± 0.15	eV	NIST Webbook
ea	4.59 ± 0.25	eV	NIST Webbook
ea	2.40	eV	NIST Webbook
ea	2.39	eV	NIST Webbook
ie	14.40	eV	NIST Webbook
log10ws	-0.35		Crippen Method
logp	0.100		Crippen Method
mcvol	43.760	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C12543758&Units=SI>

## Legend

**ea:** Electron affinity  
**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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