

Ethynyl radical

Inchi: InChI=1S/C2H/c1-2/h1H
InchiKey: XEHVFKKSDRMODV-UHFFFAOYSA-N
Formula: C2H
SMILES: [C]#C
Mol. weight [g/mol]: 25.03
CAS: 2122-48-7

Physical Properties

Property code	Value	Unit	Source
affp	753.00	kJ/mol	NIST Webbook
basg	720.80	kJ/mol	NIST Webbook
ea	2.10 ± 0.30	eV	NIST Webbook
ea	2.65	eV	NIST Webbook
ea	2.97 ± 0.00	eV	NIST Webbook
ea	2.97 ± 0.01	eV	NIST Webbook
ea	2.96 ± 0.02	eV	NIST Webbook
ea	2.94 ± 0.10	eV	NIST Webbook
ea	2.30 ± 0.70	eV	NIST Webbook
ea	3.73 ± 0.05	eV	NIST Webbook
ea	2.80	eV	NIST Webbook
hf	556.00 ± 8.00	kJ/mol	NIST Webbook
ie	11.96 ± 0.05	eV	NIST Webbook
ie	11.61 ± 0.07	eV	NIST Webbook
ie	11.61 ± 0.07	eV	NIST Webbook
ie	11.70	eV	NIST Webbook
ie	11.31 ± 0.13	eV	NIST Webbook
ie	11.51	eV	NIST Webbook
ie	11.96 ± 0.05	eV	NIST Webbook
ie	11.60 ± 0.50	eV	NIST Webbook
log10ws	-0.06		Crippen Method
logp	0.206		Crippen Method
mcvol	28.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2122487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/49-828-9/Ethynyl-radical.pdf>

Generated by Cheméo on 2024-04-18 06:56:14.549455719 +0000 UTC m=+15712623.470033034.

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