

Hydrogen isocyanide

Inchi: InChI=1S/CHN/c1-2/h2H
InchiKey: QIUBLANJVAOHY-UHFFFAOYSA-N
Formula: CHN
SMILES: [C]=N
Mol. weight [g/mol]: 27.03
CAS: 6914-07-4

Physical Properties

Property code	Value	Unit	Source
affp	772.30	kJ/mol	NIST Webbook
basg	739.80	kJ/mol	NIST Webbook
ie	12.50 ± 0.10	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	0.020		Crippen Method
mcvol	26.330	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C6914074&Units=SI>

Legend

affp: Proton affinity
basg: Gas basicity
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/44-415-2/Hydrogen-isocyanide.pdf>

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