

HCCN radical

Inchi: InChI=1S/C2HN/c1-2-3/h1H
InchiKey: SZICEGNEOSKVLO-UHFFFAOYSA-N
Formula: C2HN
SMILES: [CH]C#N
Mol. weight [g/mol]: 39.04
CAS: 2612-62-6

Physical Properties

Property code	Value	Unit	Source
ea	1.10	eV	NIST Webbook
ea	2.00 ± 0.01	eV	NIST Webbook
ea	1.88 ± 0.01	eV	NIST Webbook
ea	2.01 ± 0.34	eV	NIST Webbook
ea	1.93 ± 0.34	eV	NIST Webbook
ea	0.80 ± 0.40	eV	NIST Webbook
log10ws	-0.08		Crippen Method
logp	0.221		Crippen Method
mcpol	36.120	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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2612626&Units=SI>

Legend

ea: Electron affinity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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