

CNN Radical

Inchi:	InChI=1S/CN2/c1-3-2
InchiKey:	QDZARNQKIZUXDK-UHFFFAOYSA-N
Formula:	CN2
SMILES:	[C]=[N+]=[N-]
Mol. weight [g/mol]:	40.02
CAS:	2468-81-7

Physical Properties

Property code	Value	Unit	Source
ea	1.76 ± 0.01	eV	NIST Webbook
log10ws	-1.77		Crippen Method
logp	-0.329		Crippen Method
mcvol	32.010	ml/mol	McGowan Method

Sources

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=C2468817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

ea:	Electron affinity
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/69-487-6/CNN-Radical.pdf>

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