Isocyanato radical

Inchi: InChI=1S/CNO/c2-1-3
InchiKey: HKKDKUMUWRTAIA-UHFFFAOYSA-N
Formula: CNO
SMILES: [N]=C=O
Mol. weight [g/mol]: 42.02
CAS: 22400-26-6

Physical Properties

Property code	Value	Unit	Source
ea	3.61 ± 0.01	eV	NIST Webbook
ea	3.45 ± 0.10	eV	NIST Webbook
ea	3.80 ± 0.20	eV	NIST Webbook
ea	2.60 ± 0.40	eV	NIST Webbook
ie	11.76 ± 0.01	eV	NIST Webbook
ie	11.76 ± 0.01	eV	NIST Webbook
ie	11.76 ± 0.01	eV	NIST Webbook
log10ws	0.70		Crippen Method
logp	-0.878		Crippen Method
mcvol	30.050	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22400266&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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