

Nitrogen trioxide

Inchi: InChI=1S/NO3/c2-1(3)4
InchiKey: YPJKMVATUPSWOH-UHFFFAOYSA-N
Formula: NO₃
SMILES: [O][N+](=O)[O-]
Mol. weight [g/mol]: 62.00
CAS: 12033-49-7

Physical Properties

Property code	Value	Unit	Source
ea	3.94 ± 0.01	eV	NIST Webbook
ea	3.94 ± 0.02	eV	NIST Webbook
ea	3.70 ± 0.20	eV	NIST Webbook
ie	12.57 ± 0.03	eV	NIST Webbook
log10ws	-4.79		Crippen Method
logp	-0.391		Crippen Method
mcvol	32.000	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=C12033497&Units=SI>

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

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<https://www.cheméo.com/cid/14-472-2/Nitrogen-trioxide.pdf>

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