Methanamine, N,N-dimethyl-, N-oxide

Other names:	N,N-dimethylmethanamine N-oxide
	TMAO
	Triox
	trimethylamine oxide
	trimethylamine, N-oxide
Inchi:	InChI=1S/C3H9NO/c1-4(2,3)5/h1-3H3
InchiKey:	UYPYRKYUKCHHIB-UHFFFAOYSA-N
Formula:	C3H9NO
SMILES:	C[N+](C)(C)[O-]
Mol. weight [g/mol]:	75.11
CAS:	1184-78-7

Physical Properties

Property code	Value	Unit	Source
affp	983.20	kJ/mol	NIST Webbook
basg	953.50	kJ/mol	NIST Webbook
ie	8.38 ± 0.04	eV	NIST Webbook
ie	8.27	eV	NIST Webbook
log10ws	0.34		Crippen Method
logp	0.190		Crippen Method
mcvol	68.980	ml/mol	McGowan Method

Sources

Thermodynamics of the interactions of a homologous series of some amino acids with trimethylamine N-oxide:	https://www.doi.org/10.1016/j.jct.2011.05.012
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric, compressibility, and calorimetric studies.	
Compatible solutes: Thermodynamic properties relevant for effective protection against osmotic stress:	https://www.doi.org/10.1016/j.fluid.2015.07.004
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Interactions of some short peptides with the osmolyte trimethylamine N-oxide in aqueous solution:	https://www.doi.org/10.1016/j.jct.2011.12.029
Counteracting effects of trimethylamine N-oxide and betaine on the denaturation of urea with zwitterionic glycine peptides:	https://www.doi.org/10.1016/j.tca.2009.02.017
Unique chemical insights.	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1184787&Units=SI
Density and Volumetric Properties of Aqueous Solutions of Trimethylamine N-Oxide in the Temperature Range from (278.15 to 328.15) K and at Pressures up to 100 MPa:	https://www.doi.org/10.1021/je500977g
The hydration of the protein stabilizing agents Trimethylamine-N-oxide, glycine and its N-methylderivatives	https://www.doi.org/10.1016/j.jct.2013.01.023
The volumetric and compressibility studies:	

Physicochemical properties of L-carnitine in aqueous solution and its interaction with trimethylamine N-oxide, sodium chloride and dextrose: Volumetric and calorimetric insights: https://www.doi.org/10.1016/j.jct.2018.01.021

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