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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
Physicochemical properties of L-carnitine in aqueous solution and its counteracting effects on trimethylamine N-oxide and urea:	https://www.doi.org/10.1016/j.jct.2018.01.021
Calorimetric studies of trimethylamine N-oxide aqueous mixtures with zwitterionic glycine peptides:	https://www.doi.org/10.1016/j.tca.2009.02.017
Volumetric and calorimetric insights:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1184787&Units=SI
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
Density and Volumetric Properties of Aqueous Solutions of Trimethylamine N-Oxide in the Temperature Range from (278.15 to 323.15) K and at Pressures up to 100 MPa:	https://www.doi.org/10.1021/je500977g

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

Latest version available from: