

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	8.27	eV	NIST Webbook
ie	8.38 ± 0.04	eV	NIST Webbook
log10ws	0.34		Crippen Method
logp	0.190		Crippen Method
mcvol	68.980	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1184787&Units=SI>

The hydration of the protein stabilizing agents: Trimethylamine-N-oxide, Density and Volumetric Properties of Aqueous Solutions of Trimethylamine N-oxide in the Temperature Range 278.15-318.15 K and at Pressures up to 100 MPa: thermodynamic properties relevant for effective protection against osmotic stress: <https://www.doi.org/10.1016/j.jct.2013.01.023>

Interactions of some short peptides with the osmolyte trimethylamine N-oxide in aqueous solution: physico-chemical insights: <https://www.doi.org/10.1021/je500977g>

McGowan Method: <https://www.doi.org/10.1016/j.tca.2009.02.017>

Crippen Method: <https://www.doi.org/10.1016/j.fluid.2015.07.004>

Thermodynamics of the interactions of a homologous series of some amino acids with trimethylamine N-oxide: Volumetric, compressibility, and calorimetric studies: https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1016/j.jct.2011.12.029>

<http://link.springer.com/article/10.1007/BF02311772>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.doi.org/10.1016/j.jct.2011.05.012>

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

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