

1-Methyl-2,4,5-trioxoimidazolidine

Other names:	Methylparabanic acid Imidazolidinetrione,methyl-
Inchi:	InChI=1S/C4H4N2O3/c1-6-3(8)2(7)5-4(6)9/h1H3,(H,5,7,9)
InchiKey:	MJJCZWPYKMGQHU-UHFFFAOYSA-N
Formula:	C4H4N2O3
SMILES:	CN1C(=O)NC(=O)C1=O
Mol. weight [g/mol]:	128.09
CAS:	3659-97-0

Physical Properties

Property code	Value	Unit	Source
ie	10.52	eV	NIST Webbook
log10ws	0.55		Crippen Method
logp	-1.305		Crippen Method
mcvol	81.030	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=C3659970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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:

<https://www.cheméo.com/cid/113-287-8/1-Methyl-2-4-5-trioxoimidazolidine.pdf>

Generated by Cheméo on 2024-04-30 17:42:22.98732863 +0000 UTC m=+16788191.907905945.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.